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(54) Title: CRYSTAL STRUCTURE OF A DEACETYLASE AND INHIBITORS THEREOF

(57) Abstract: The present invention provides three-dimensional structural information from the hyperthermophilic bacterium Aquifex aeolicus which is a histone deacetylase-like protein (HDLP). HDLP shares 35.2% amino acid sequence identity with human histone deacetylase (HDAC1). The present invention further provides three-dimensional structural information of HDLP bound by inhibitor molecules. The three-dimensional structural information of the present invention is useful to design, isolate and screen deacetylase inhibitor compounds capable of inhibiting HDLP, HDAC family members and HDLP-related molecules. The invention also relates to nucleic acids encoding a mutant HDLP which facilitates the determination of the three-dimensional structure of HDLP in the presence of a zinc atom.



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Crystal Structure of a Deacetylase and Inhibitors Thereof

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This application claims priority of U.S. Provisional Application No. 60/152,753, filed September 8, 1999, the contents of which are hereby incorporated by reference.

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This invention has been made with government support under National Institutes of Health Grant No. RO1 CA-65698. Accordingly, the U.S. Government may have certain rights in the invention.

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Throughout this application, various publications are referenced by author, date and citation. The disclosures of these publications in their entireties are hereby incorporated by reference into this application in order to more fully describe the state of the art as known to those skilled therein as of the date of the invention described and claimed herein.

Introduction

25 The present invention relates to a histone deacetylase homologue from the hyperthermophilic bacterium Aquifex aeolicus, HDLP (histone deacetylase like protein; also known as AcuCl), which shares 35.2 % sequence identity with human histone deacetylase (HDACl), that can be co-crystallized with an inhibitory ligand, and more particularly, to the detailed crystallographic data obtained from said co-crystallization which is disclosed herein. The invention also relates to methods of using the crystal structure and x-ray crystallographic coordinates of the apo-HDLP and

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inhibitor-bound HDLP to design, isolate and screen compounds which bind to and inhibit the active site of HDLP and HDLP-related proteins, such as those proteins belonging to the HDAC family, including HDAC1.

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Background of the Invention

The reversible modification of histones by acetylation is associated with changes in nucleosome conformation and chromatin structure, and plays an important role in the regulation of gene expression (reviewed in Davie and Chadee, 1998, J. Cell Biochem. Suppl. 30-31:203-213). The histone acetylase and deacetylase enzymes that carry out these modifications are involved in many cellular processes such as cell cycle progression and differentiation, and their deregulation is associated with several types of human cancer (reviewed in Kouzarides, 1999, Curr. Opin. Genet. Dev. 9:40-48; Hassig et al., 1997, Chem. Biol. 4:783-789; Fenrick and Heibert, 1998, J. Cell. Biochem. Suppl. 30-31:194-202).

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Recently, several experimental antitumor compounds, such as trichostatin A (TSA), trapoxin, suberoylanilide hydroxamic acid (SAHA), and phenylbutyrate have been shown to act, at least in part, by inhibiting histone deacetylases. Richon et al., 1998, Proc. Natl. Acad. Sci., USA 95:3003-3007; Yoshida et al., 1990, J. Biol. Chem. 265:17174-17179; Kijima et al., 1993, J. Biol. Chem. 268:22429-22435. Additionally, diallyl sulfide and related molecules (Lea et al., 1999, Int. J. Oncol. 2:347-352), oxamflatin (Kim et al., 1999, Oncogene 15:2461-2470), MS-27-275, a synthetic benzamide derivative (Saito et al., 1999, Proc. Natl. Acad. Sci. 96:4592-4597),

butarate derivatives (Lea and Tulsyan, 1995, Anticancer Res. 15:879-883), FR901228 (Nokajima et al., 1998, Exp. Cell Res. 241:126-133), depudecin (Kwon et al., 1998, Proc. Natl. Acad. Sci. USA 95:3356-3361) and m-carboxysinnamic acid bishydroxamide (CBHA; Richon et al., Proc. Natl. Acad. Sci. USA 95:3003-3007) have been shown to inhibit histone deacetylases. In vitro, these compounds can inhibit the growth of fibroblast cells by causing cell cycle arrest in the G1 and G2 phases (Richon et al., 1996, Proc. Natl. Acad. USA 93:5705-5708; Kim et al., 1999, Oncogene 18:2461-2470; Yoshida et al., 1995, Bioessays 17:423-430; Yoshida & Beppu, 1988, Exp. Cell. Res. 177:122-131), and can terminal differentiation and loss to the transforming potential of a variety of transformed cell lines. Richon et al., 1996, Proc. Natl. Acad. Sci. USA 93:5705-5708; Kim et al., 1999, Oncogene 18:2461-2470; Yoshida et al., 1987, Cancer Res. 47:3688-3691. phenylbutyrate is effective in the treatment of acute promyelocytic leukemia in conjunction with retinoic acid. Warrell et al., 1998, J. Natl. Cancer Inst. 90:1621-1625. SAHA is effective in preventing the formation of mammary tumors in rats, and lung tumors in mice. Desai et al., 1999, Proc. AACR 40: abstract #2396; Cohen et al., Cancer Res., submitted.

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Histone deacetylases catalyze the removal of acetyl groups from the e-amino groups of lysine residues clustered near the N-terminus of nucleosomal histones, and this process is associated with transcriptional repression (reviewed in Struhl, 1998, Genes Dev. 12:599-606). Deletion of the yeast histone deacetylase gene, rpd3, or its pharmacological

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inactivation with trichostatin A reduces the transcriptional repression in a subset of promoters, such as those of Ume6-regulated genes. Kadosh & Struhl, 1998, Mol. Cell. Biol. 18:5121-5127. This is accompanied by the increased acetylation of H4 histones in the repressed promoter and its vicinity, but has no effect on histones at promoter distal regions. Kadosh & Struhl, 1998, Mol. Cell. Biol. 18:5121-5127; Rundlett et al., 1998, Nature 392:831-835.

Histone deacetylases are recruited to specific promoters by associating with DNA-binding transcriptional repressors, either directly or through co-repressors that bridge the deacetylase to the transcriptional repressors. For example, the Mad and Ume6 repressors bind to the co-repressor Sin3A (Laherty et al., 1997, Cell 89:349-356; Hassig et al., 1997, Cell 89:341-347; Kadosh & Struhl, 1997, Cell 89:365-371), and the nuclear receptors bind N-CoR and the related SMRT co-repressors. Nagy et al., 1997, Cell 89:373-380; Alland et al, 1997, Nature 387:49-55; Heinzel et al, 1997, Nature 387:43-48.

The deregulation of histone deacetylase recruitment appears to be one of the mechanisms through which these enzymes contribute to tumorigenesis. In acute promyelocytic leukemia (APL), chromosomal translocations fuse the retinoic acid receptor- α (RAR α) to either PLZF or to PML. These fusion oncoproteins have aberrant transcriptional repression activity resulting, in part, through the recruitment of a co-repressor and, in turn, HDACs. Grignani et al, 1998, Nature 391:815-818; Lin et al., 1998, Nature 391:811-814. Treatment of PLZF-RAR α APL cells with TSA enhances their

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responsiveness to retinoic acid-induced differentiation. Grignani et al, 1998, Nature 391:815-818; Lin et al., 1998, Nature 391:811-814.

5 The histone deacetylases comprise a large family of proteins, conserved from yeast to man, and are divided into two related classes. Class I is characterized by human HDAC1, 2, 3 (Taunton et al., 1996, Science 272:408-411; Yang et al., 1996, Proc. Natl. Acad. Sci. USA 93:12845-12850; 10 Emiliani et al., 1998, Proc. Natl. Acad. Sci. USA 95:2795-2800), and yeast RPD3 (Videl & Gaber, 1991, Mol. Cell. Biol. 11:6317-6327), and class II by the human HDAC4, 5, 6 (Grozinger et al., 1999, Proc. Natl. Acad. Sci. USA 96:4868-4873; Fischle, et al., 1999, J. Biol. Chem. 274:11713-15 11720), and yeast HDA1 (Rundlett et al., 1996, Proc. Natl. Acad. Sci. USA 93:14503-14508). The two classes share a ~390 amino acid region of sequence similarity, comprising the deacetylase core, but are divergent outside this region. The histone deacetylase genes belong to an even larger 20 superfamily (Leipe & Landsman, 1997, Nucleic Acids Res. 25:3693-3697) that contains the prokaryotic utilization proteins (AcuC; 28.1% sequence identity to HDAC1), and the prokaryotic acetylpolyamine amidohydrolases (APAH; 15.0 % sequence identity to HDAC1). The enzymatic activity of AcuC is not clear, but its disruption reduces 25 the ability of B. subtilis to breakdown acetoin and utilize it as a carbon source. Grundy et al., 1993, Mol. Microbiol. 10:259-271. APAHs catalyze the deacetylation of polyamines by cleaving a non-peptide amide bond (reviewed in Leipe & Landsman, 1997, Nucleic Acids Res. 25:3693-3697). 30

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It is useful to address the questions of how HDACs and HDACrelated proteins catalyze the deacetylation of histones and how the above-referenced compounds, particularly those compounds with antitumor activity, inhibit this activity in order to better understand the mechanism of inhibition of HDACs and to facilitate discovery of additional useful compounds which may inhibit this activity. To this end, the present invention has determined the three dimensional structure of a HDAC1-like protein from the thermophilic bacterium Aquifex aeolicus, herein after HDLP. determination of the nucleic acid coding sequence of HDLP was described by Deckert et al., 1998, Nature 392:353-358. encoded 375 residue protein, whose sequence was The determined from the nucleic acid encoding sequence, shares 35.2% amino acid sequence identity with HDAC1, deacetylates histones in vitro, and is inhibited by TSA, SAHA and several other HDAC inhibitors. The determination of the threedimensional structure of HDLP is useful in the design, identification and screening of new HDAC family inhibitory compounds which are useful for the inhibition of cell growth both in vivo and in vitro.

Summary of the Invention

In general, it is the object of the present invention to provide detailed three-dimensional structural information for a family of proteins known as histone deacetylases (HDAC), and particularly a homologue from the hyperthermophilic bacterium Aquifex aeolicus HDLP (histone deacetylase-like protein) which shares 35.2 % sequence identity with human histone deacetylase (HDAC1). It is also an object of the present invention to provide three-

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dimensional structural information of an HDLP bound to an inhibitory compound.

In one embodiment of the invention, three-dimensional structure information is obtained from a crystal of wildtype HDLP (SEQ ID NO:1) (the nucleic acid encoding wild-type In a further embodiment of the HDLP is SEQ ID NO:2). invention, three-dimensional information is obtained from a mutant HDLP comprising two mutations (1) cysteine 75 to a serine and (2) cysteine 77 to a serine (Cys75Ser/Cys77Ser double mutant; SEQ ID NO:3) (the nucleic acid encoding HDLP Cys75Ser/Cys77Ser double mutant is SEQ ID NO:4). The HDLP of the invention mutant present facilitates the determination of three-dimensional structural information of HDLP bound to a zinc atom at its zinc atom-binding site.

In a preferred embodiment of the invention, the threedimensional structural information is obtained from a cocrystal of a protein-inhibitor compound complex that comprises HDLP or HDLP Cys75Ser/Cys77Ser double mutant and trichostatin A (TSA). In another preferred embodiment of the invention the three-dimensional structural information is obtained from a co-crystal of a protein-inhibitor compound complex that comprises HDLP or HDLP Cys75Ser/Cys77Ser suberoylanilide double mutant and hydroxamic acid (SAHA). Any HDLP or HDLP-related protein (e.g. HDAC) inhibitor compound that may be co-crystallized with HDLP may be used to form a co-crystal of the present invention.

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The protein crystals and protein-inhibitory complex cocrystals of the present invention diffract to a high 5

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resolution limit of at least equal to or greater than 4 angstrom (Å). In a preferred embodiment, the protein crystals and protein-inhibitory complex co-crystals of the present invention diffract to a high resolution limit of greater than 2.5 Å.

A crystal of the present invention may take a variety of forms, all of which are contemplated by the present invention. In a preferred embodiment, the crystal has a space group of C2 with one molecule in the asymmetric unit and with unit dimensions of a = 51.4 Å, b = 93.8 Å, 78.7 Å and β = 96.9° (see, e.g., Example 2, below). another preferred embodiment, the crystal has a space group of $P2_12_12_1$ with two molecules in the asymmetric unit and with unit dimensions of a=53.4 Å, b=94.4 Å, c=156.3 Å (see, e.g., Example 2, below). The HDLP structure comprises a parallel β sheet with α helices packing against both faces. At one end of the β sheet, the HDLP has a narrow, tube-like pocket formed by several well-ordered loops. The walls of the pocket are lined with hydrophobic residues and there is a zinc binding site and several polar side chains at the bottom of the pocket. The inhibitory compounds of the present invention bind in the pocket.

The three-dimensional structural information obtained from crystals of HDLP, HDLP Cys75Ser/Cys77Ser double mutant, HDLP Cys75Ser/Cys77Ser double mutant comprising a zinc atom, HDLP comprising an inhibitory compound such as TSA or SAHA, and HDLP Cys75Ser/Cys77Ser double mutant comprising an inhibitor compound such as TSA or SAHA may be employed to solve the structure of any HDLP-related protein (e.g. HDAC) crystal,

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or any mutant HDLP-related protein and particularly any wild type or mutant of HDLP-related protein complexed with a ligand, including a substrate or inhibitor compound. If the crystals are in a different space group than the known structure, molecular replacement may be employed to solve the structure, or if the crystals are in the same space group, refinement and difference fourier methods may be employed. The structure of HDLP-related proteins (e.g. HDAC1) comprise no greater than a 2.0 Å root mean square deviation (rmsd) in the positions of the Ca atoms for at least 50% or more of the amino acids of the full-length HDLP structure.

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The present invention also provides a nucleic acid molecule encoding an HDLP Cys75Ser/Cys77Ser double mutant having the amino acid sequence of SEQ ID NO:3 and the nucleic acid sequence of SEQ ID NO:4. It is also contemplated by the invention that mutations be made in HDLP-related proteins at cysteine residues, as with the Cys75Ser/Cys77Ser double mutant, in order to facilitate the determination of the structure of said proteins bound to a zinc atom. Additionally, the present invention provides expression vectors which comprise the nucleic acid molecule encoding an HDLP Cys75Ser/Cys77Ser double mutant encoded by the sequence represented by SEQ ID NO:4 operatively linked to expression control sequences.

It is another object of the present invention to provide methods for the design, identification and screening of potential inhibitor compounds of the HDLP/HDAC family. In a preferred embodiment the method for the rational design,

identification and screening of potential inhibitor compounds for HDLP and HDLP-related proteins (e.g. HDACs) comprising deacetylase activity comprises the steps of: (a) using a three-dimensional structure of an HDLP as defined by the atomic coordinates of the present invention; employing said three-dimensional structure to design or select said potential inhibitor compound; (c) synthesizing and/or selecting said potential inhibitor; (d) contacting said potential inhibitor compound with said enzyme in the presence of acetylated substrate; and (e) determining the percent inhibition of deacetylase activity to determine the inhibitory activity of said potential inhibitor compound. In a further preferred embodiment, the binding properties of said rationally designed inhibitory compound may be determined by a method comprising the steps of: (a) forming a complex comprising said inhibitory compound and HDLP or a HDLP-related protein, (b) co-crystallizing said inhibitory compound-HDLP complex; (c) determining said dimensional structure of said co-crystal through molecular replacement or refinement and difference fourier with the molecular coordinates of HDLP as defined by the present invention; and (d) analyzing the three-dimensional structure to determine the binding characteristics of said potential inhibitor compound.

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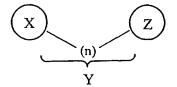
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It is a further object of the present invention to identify a defined class of HDLP/HDAC family inhibitor compounds. The HDLP/HDAC family inhibitor compounds of the present invention are represented by formula (I):

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(I)



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wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of proline and leucine; Y comprises an aliphatic chain group which binds to at least one amino acid selected from the group consisting of leucine, phenylalanine and glycine; and Z comprises and active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and may further bind to a zinc atom.

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Brief Description of the Drawings

Figure 1 is a table listing the statistics from the X-ray crystallographic analysis of a HDLP crystal, a HDLP-TSA co-crystal, and a HDLP-SAHA co-crystal.

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Figure 2 shows an alignment of various HDAC homologues with percent sequence identity depicted.

Figure 3 shows a graph indicating the histone deacetylase activity of HDLP and HDAC1 and the inhibition of HDLP and HDAC1 by the inhibitors TSA and HC-toxin.

Figure 4 shows (A & B) a schematic representation of the HDLP-Zn²⁺-TSA complex in two approximately orthogonal views,

(C) a topology diagram of HDLP indicating the regions of homology with HDAC1, and (D) a close-up schematic representation of the HDLP-Zn²⁺-SAHA complex.

Figure 5 shows (A) a schematic representation of a slice through a surface representation of HDLP with the pocket internal cavities and position of the β sheet indicated, (B) a schematic representation of a close-up view of the active site looking down into the pocket in an orientation similar to Figure 4B.

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Figure 6 shows (A) a space-filling representation of TSA in the active site pocket, (B) a closeup stereo view of the structure of the HDLP-ZN²⁺-TSA complex in a similar orientation to Figure 4B, and (C) a schematic representation of the HDLP-TSA interactions.

Figure 7 shows (A) a schematic representation of the regions of homology shared between HDLP and HDAC1 in an orientation similar to that of Figure 4A, and (B) a detailed schematic representation of the homology shared in the pocket and internal cavity between HDLP and HDAC1 in an orientation similar to that of Figure 4B.

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Figure 8 shows a schematic representation of the proposed catalytic mechanism for the deacetylation of acetylated lysine.

Figure 9 shows a schematic representation of a space filling diagram showing the conserved amino acids in the active site and nearby grooves.

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Figure 10 is the nucleic acid sequence of HDLP from Aquifex aeolicus (SEQ ID NO. 2).

Figure 11 is the amino acid sequence of full length HDLP from Aquifex aeolicus (SEQ ID NO. 1).

Figure 12 is the nucleic acid sequence of the HDLP active site mutant Tyr297Phe (SEQ ID NO. 6).

25 **Figure 13** is the amino acid sequence of the HDLP active site mutant Tyr297Phe (SEQ ID NO. 5).

Figure 14 is the nucleic acid sequence of a double mutant of HDLP from Aquifex aeolicus comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO. 4).

Figure 15 is the amino acid sequence of a double mutant of HDLP from Aquifex aeolicus comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO. 3).

- Figure 16-1 to 16-49 lists the atomic structure coordinates for HDLP as derived by X-ray diffraction from a crystal of HDLP.
- Figure 17-1 to 17-49 lists the atomic structure coordinates

 for HDLP Cys75Ser/Cys77Ser double mutant comprising a zinc
 atom in the active site as derived by X-ray diffraction from
 a crystal of the HDLP Cys75Ser/Cys77Ser double mutant.
- Figure 18-1 to 18-99 lists the atomic structure coordinates

 for HDLP Cys75Ser/Cys77Ser double mutant as derived by X-ray
 diffraction from a co-crystal of HDLP complexed with TSA.
- Figure 19-1 to 19-48 lists the atomic structure coordinates for HDLP Cys75Ser/Cys77Ser double mutant as derived by X-ray diffraction from a co-crystal of HDLP complexed with SAHA.

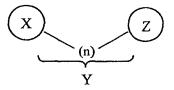
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Detailed Description of the Invention

The present invention provides crystals of a histone deacetylase (HDAC) homologue grown in the presence and absence of a compound capable of inhibiting the histone deacetylase activity of said HDAC homologue. As referred to herein, a HDAC homologue (as well as a HDLP-related protein) is any protein molecule having (a) greater than 15% sequence identity to over the 375 amino acid residues of HDLP; (b) having no more than twenty insertions or deletions for a total of no more than 100 amino acids; and (c) deacetylase activity. Sequence identity is calculated by the program DNAstar^M using the identity matrix weighing scheme clustal method (DNAstar program, Madison, WI).

A HDLP/HDAC inhibitor compound, as used herein, refers to any compound represented by Formula (I):

(I)



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wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of tyrosine, proline and leucine; Y comprises an aliphatic chain group from about 5 to about 10 Å, preferably 7 Å, which binds to at least one amino acid selected from the group consisting of phenylalanine and glycine; and Z comprises a active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and which may further bind to a zinc atom. The HDAC inhibitory compounds of the present

invention can inhibit greater than 50% of the histone deacetylase activity of a HDAC homologue or a HDLP-related protein.

To grow the crystals of the present invention, the HDAC and HDAC-inhibitory compound complex are purified to greater than 80% total protein and more preferably purified to greater than 90% total protein. For expression and purification purposes, the full-length HDLP (Genbank accession number AE000719) may be subcloned from Aquifex aeolicus chromosomal DNA preparation by the polymerase chain reaction (PCR) and inserted into an expression vector.

A large number of vector-host systems known in the art may be used. Possible vectors include, but are not limited to, 15 plasmids or modified viruses, but the vector system must be compatible with the host cell used. Examples of vectors include E. coli bacteriophages such as lambda derivatives, or plasmids such as pBR322 derivatives or pUC plasmid 20 derivatives, e.q., pGEX vectors (Amersham-Pharmacia, Piscataway, New Jersey), pET vectors (Novagen, Madison, WI), pmal-c vectors (Amersham-Pharmacia, Piscataway, New Jersey), pFLAG vectors (Chiang and Roeder, 1993, Pept. Res. 6:62-64), baculovirus vectors (Invitrogen, Carlsbad, CA; Pharmingen, 25 San Diego, CA), etc. The insertion into a cloning vector can, for example, be accomplished by ligating the DNA fragment into a cloning vector which has complementary cohesive termini, by blunt end ligation if no complementary cohesive termini are available or by through nucleotide linkers using techniques standard in the art. 30 Ausubel et al. (eds.), Current Protocols in Molecular

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Biology, (1992). Recombinant vectors comprising the nucleic acid of interest may then be introduced into a host cell compatible with the vector (e.g. E. coli, insect cells, mammalian cells, etc.) via transformation, transfection, infection, electroporation, etc. The nucleic acid may also be placed in a shuttle vector which may be cloned and propagated to large quantities in bacteria and then introduced into a eukaryotic cell host for expression. The vector systems of the present invention may provide expression control sequences and may allow for the expression of proteins in vitro.

In a preferred embodiment, the full length HDLP (SEQ ID NO:2) is subcloned from Aquifex aeolicus chromosomal DNA preparation into pGEX4T3 (Amersham-Pharmacia, Piscataway, New Jersey). In order to construct a double mutant comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO:4), and to construct the HDLP active site mutant Tyr297Phe (SEQ ID NO:5 and SEQ ID NO:6), PCR site directed mutagenesis may be employed with verification by DNA sequencing by methods known to those skilled in the art (see, e.g., Exemple 1 below). The mutants of the present invention may be subcloned into a suitable expression vector and introduced into a host cell for protein production, as described above.

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The HDLP nucleic acids of the present invention may be subcloned into an expression vector to create an expression construct such that the resultant HDLP molecule which is produced comprises a fusion protein wherein said fusion protein comprises a tag for ease of purification. As referred to herein, a "tag" is any additional amino acids

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which are provided in a protein either c-terminally, nterminally or internally for the ease of purification, for the improvement of production or for any other purpose which may facilitate the goals of the present invention (e.g. to achieve higher levels of production and/or purification). Such tags include tags known to those skilled in the art to be useful in purification such as, but not limited to, his tag, glutathione-s-transferase tag, flag tag, mbp (maltose binding protein) tag, etc. In a preferred embodiment, the wild-type and mutant HDLPs of the present invention are tagged with glutathione-s-transferase (see Example 1 below). In another preferred embodiment, HDAC1 is flag tagged (see Example 1 below). Such tagged proteins may also be engineered to comprise a cleavage site, such as a thrombin, enterokinase or factor X cleavage site, for ease of removal of the tag before, during or after purification. systems which provide a tag and a cleavage site for removal of the tag are particularly useful to make the expression constructs of the present invention.

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The tagged HDLPs and HDACs of the present invention may be purified by immuno-affinity or conventional chromatography, including but not limited to, chromatography employing the following: glutathione-sepharose™ (Amersham-Pharmacia, Piscataway, New Jersey) or an equivalent resin, nickel or cobalt-purification resins, anion exchange chromatography, cation exchange chromatography, hydrophobic resins, gel filtration. antiflag epitope resin, reverse chromatography, etc. After purification, the HDLP and HDLPinhibitor compound complex may be concentrated to greater than 1 mg/ml for crystallization purposes. In a preferred embodiment HDLP and HDLP-inhibitor complexes

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concentrated to greater than 10 mg/ml for crystallization and in a particularly preferred embodiment, HDLP and HDLP-inhibitor complexes are concentrated to greater than 20 mg/ml.

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In order to determine whether the purified HDLPs of the present invention demonstrate histone deacetylase activity, the purified HDLPs and also any HDLP-related protein may be assayed by any method known to those skilled in the art for the determination of said activity. In a preferred embodiment, the purified HDLPs of the present invention are incubated in the presence of [3H] acetyl-labeled histone substrate (Carmen et al., 1996, J. Biol. Chem. 271:15837-15844) in a buffer suitable for detection of histone deacetylase activity (see Example 3 below); stopping the reaction; extracting the released acetate and measuring said released acetate, as described by Henzel et al. (J. Biol. Chem. 266:21936-21942 (1991); Example 3 below). preferred embodiment, the HDLPs of the present invention are inclubated in the presence of ZnCl2 in order to obtain histone deacetylase activity therefrom (Example 3 below).

In another embodiment, the crystals of the present invention comprise purified wild-type HDLP (SEQ ID NO:1) and are grown at room temperature by the hanging-drop vapor-diffusion method from a crystallization solution comprising one or more precipitants selected from the group consisting of isopropanol, polyethylene glycol, and tert butanol (see Example 2 below). The crystallization solution may further comprise one or more salts including salts selected from the group consisting of NaCl and KCl, and one or more buffers

including buffers selected from the group consisting of Tris (tris(hydroxymethyl)aminomethane and bis-tris propane-Cl (1,3-bis[tris(hydroxymethyl)methyl-amino] propane) (see Example 2 below). The pH of the crystallization solution is preferably between pH 5 to 9, although other pH values are also contemplated by the present invention (see Example 2 below).

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Any crystallization technique known to those skilled in the art may be employed to obtain the crystals of the present invention, including, but not limited to, batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and micro dialysis. Seeding of the crystals in some instances may be required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used.

The crystals of the present invention may form in the space group C2 with one molecule in the asymmetric unit and with unit dimensions of a=51.4 Å, b=93.8 Å, c=78.7 Å and $\beta=96.9^{\circ}$ (see Example 2 below). The crystals of the present invention may also form in the space group $P2_12_12_1$ with two molecules in the asymmetric unit and with unit dimensions of a=53.4 Å, b=94.4 Å, c=156.3 Å (see Example 2 below). However, the present invention contemplates crystals which form in any space group including, but not limited to, C2, $P2_1$, $P2_12_12_1$, $P3_121$, $P4_32_12_1$, and $C222_1$. The crystals diffract to a resolution greater than 4 Å, preferably greater than 2.5 Å.

To collect diffraction data from the crystals of the present

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invention, the crystals may be flash-frozen in crystallization buffer employed for the growth of said crystals, however with preferably higher precipitant concentration (see, e.g., Example 2 below). For example, but not by way of limitation, if the precipitant used was 28% PEG 1500, the crystals may be flash frozen in the same crystallization solution employed for said crystal growth wherein the concentration of the precipitant is increased to 35% (see Example 2 below). If the precipitant is not a sufficient cryoprotectant (i.e. a glass is not formed upon cryoprotectants (e.g. glycerol, low flash-freezing), molecular weight PEGs, alcohols, etc) may be added to the solution in order to achieve glass formation upon flashfreezing, providing the cryoprotectant is compatible with preserving the integrity of the crystals. The flash-frozen crystals are maintained at a temperature of less than -110°C and preferably less than -150°C during the collection of the crystallographic data by X-ray diffraction. diffraction data may be processed with DENZO and SCALEPACK (Otwinowski & Minor, 1997, Method Ensemble. 276:307-326) but any method known to those skilled in the art may be used to process the X-ray diffraction data.

In order to determine the atomic structure of HDLP according to the present invention, multiple isomorphous replacement (MIR) analysis, model building and refinement may be performed. For MIR analysis, the crystals may be soaked in heavy-atoms to produce heavy atom derivatives necessary for MIR analysis. As used herein, heavy atom derivative or derivitization refers to the method of producing a chemically modified form of a protein or protein complex

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crystal wherein said protein is specifically bound to a heavy atom within the crystal. In practice a crystal is soaked in a solution containing heavy metal atoms or salts, or organometallic compounds, e.g., lead chloride, gold cyanide, thimerosal, lead acetate, uranyl acetate, mercury chloride, gold chloride, etc, which can diffuse through the crystal and bind specifically to the protein. location(s) of the bound heavy metal atom(s) or salts can be determined by X-ray diffraction analysis of the soaked This information is used to generate MIR phase crystal. information which is used to construct the three-dimensional structure of the crystallized HDLPs and HDLP-related proteins of the present invention. In a preferred embodiment, the heavy atoms comprise thimerosal, $\text{KAu}\left(\text{CN}\right)_2$ and $Pb(Me)_3OAc$ (see Example 2 below). The MIR phases may be calculated by any program known to those skilled in the art and preferably with the program MLPHARE (The CCP4 suite: Programs for computational crystallography, 1994, Crystallogr. D. 50:760-763) and may also use the anomalous diffraction signal from the thimerosal derivative. preferred embodiment, the MIR phases were calculated at 2.5 Å and have a mean figure of merit of 0.55 (see Figure 19 and Example 2 below). The phases may be improved where necessary by solvent flattening by methods known to those skilled in the art including, but not limited to, through the use of the program DM (The CCP4 suite: Programs for computational crystallography, 1994, Acta Crystallogr. D <u>50</u>:760-763).

30 Thereafter, an initial model of the three-dimensional structure may be built using the program O (Jones et al.,

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1991, Acta Crystallogr. A <u>47</u>:110-119). The interpretation and building of the structure may be further facilitated by use of the program CNS (Brunger et al., 1998, Acta Crystallogr. D <u>54</u>:905-921).

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For the determination of the HDLP-inhibitor compound complex structure, if the space group of the HDLP-inhibitor compound complex crystal is different, molecular replacement may be employed using a known structure of apo-HDLP (as referred to herein, apo-HDLP or apo-HDAC is the enzyme which is not complexed with an inhibitor compound) or any known HDLP/inhibitor complex structure whose structure may be determined as described above and below in Example 2. Ιf the space group of the HDLP-inhibitor compound crystals is the same, then rigid body refinement and difference fourier may be employed to solve the structure using a known structure of apo-HDLP (as referred to herein, apo-HDLP or apo-HDAC is the enzyme which is not complexed with an inhibitor compound) or any known HDLP/inhibitor complex structure.

The term "molecular replacement" refers to a method that involves generating a preliminary model of the three-dimensional structure of the HDLP crystals of the present invention whose structure coordinates are unknown prior to the employment of molecular replacement. Molecular replacement is achieved by orienting and positioning a molecule whose structure coordinates are known (in this case the previously determined apo-HDLP) within the unit cell as defined by the X-ray diffraction pattern obtained from an HDLP or HDLP-related protein crystal whose structure is

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unknown so as to best account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of several forms of refinement to provide a final, accurate structure.

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Any method known to the skilled artisan may be employed to determine the structure by molecular replacement. For example, the program AMORE (The CCP4 suite: Programs for computational crystallography, 1994, Acta Crystallogr. D. 50:760-763) may be employed to determine the structure of an unknown histone deacetylase +/- an inhibitor by molecular replacement using the apo-HDLP coordinates (Figure 16). For the structure determination of the inhibitory compound TSA, the structure of TSA was obtained from the Cambridge Structural Database (Refcode TRCHST, http://www.ccdc.cam.ac.uk >>) may be employed to define the stereochemical restraints used in the refinement with the program CNS (Brunger et al., 1998, Acta Crystallogr. D <u>54</u>:905-921).

The three-dimensional structural information and the atomic coordinates associated with said structural information of HDLP are useful for solving the structure of crystallized proteins which belong to the HDAC family by molecular replacement. Similarly, any structure of a crystallized protein which is thought to be similar in structure based on function or sequence similarity or identity to HDLP may be solved by molecular replacement with the HDLP structural

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information of the present invention. The structure of HDLP-related proteins as determined by molecular replacement as described above and in Example 2 below, comprise a root mean square deviation (rmsd) of no greater than 2.0 Å in the positions of $C\alpha$ atoms for at least 50% or more of the amino acids of the structure over the 375 residues of full-length HDLP. Such a rmsd may be expected based on the amino acid sequence identity. Chothia & Lesk, 1986, Embo J. $\underline{5}$:823-826.

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The refined three-dimensional HDLP structures of the present invention, specifically apo-HDLP, Cys75Ser/Cys77Ser double mutant HDLP comprising a zinc atom in the active site, HDLP/TSA complex comprising a zinc atom in the active site, and HDLP/SAHA complex comprising a zinc atom in the active site, are represented by the atomic coordinates set forth in Figures 16 to 19 respectively. The refined model for apo-HDLP comprising amino acids 1-375 consists of wild-type HDLP residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered and was determined to a resolution Å. Similarly, the refined model Cys75Ser/Cys77Ser double mutant HDLP comprising a zinc atom in the active site also consists of residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered and was determined to a resolution of 2.0 Å. The refined model for the HDLP/TSA complex comprising a zinc atom in the active site consists of the Cys75Ser/Cys77Ser double mutant HDLP residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered, has TSA in the binding pocket and was determined to a resolution of 2.1 Å. HDLP/SAHA complex is similar to the HDLP/TSA complex but has SAHA in the binding pocket and was determined to a resolution of 2.5 Å.

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For the purposes of further describing the structure of HDLP and HDLP-related proteins, including, but not limited to, HDACs, from the data obtained from the HDLP crystals of the present invention, the definition of the following terms is provided:

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The term " β sheet" refers to two or more polypeptide chains (or β strands) that run alongside each other and are linked in a regular manner by hydrogen bonds between the main chain C=O and N-H groups. Therefore all hydrogen bonds in a beta-sheet are between different segments of polypeptide. Most β -sheets in proteins are all-parallel (protein interiors) or all-antiparallel (one side facing solvent, the other facing the hydrophobic core). Hydrogen bonds in antiparallel sheets are perpendicular to the chain direction and spaced evenly as pairs between strands. Hydrogen bonds in parallel sheets are slanted with respect to the chain direction and spaced evenly between strands.

The term " α helix" refers to the most abundant helical 20 conformation found in globular proteins. The average length of an α helix is 10 residues. In an α helix, all amide protons point toward the N-terminus and all carbonyl oxygens point toward the C-terminus. The repeating nature of the phi, psi pairs ensure this orientation. Hydrogen bonds 25 within an $\boldsymbol{\alpha}$ helix also display a repeating pattern in which the backbone C=O of residue X (wherein X refers to any amino acid) hydrogen bonds to the backbone HN of residue X+4. The α helix is a coiled structure characterized by 3.6 $\,$ residues per turn, and translating along its axis 1.5 Å per 30 amino acid. Thus the pitch is 3.6x1.5 or 5.4 Å. The screw sense of alpha helices is always right-handed.

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The term "loop" refers to any other conformation of amino acids (i.e. not a helix, strand or sheet). Additionally, a loop may contain bond interactions between amino acid side chains, but not in a repetitive, regular fashion.

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Amino acid residues in peptides shall herein after be abbreviated as follows: Phenylalanine is Phe or F; Leucine is Leu or L; Isoleucine is Ile or I; Methionine is Met or M; Valine is Val or V; Serine is Ser or S; Proline is Pro or P; Threonine is Thr or T; Alanine is Ala or A; Tyrosine is Tyr or Y; Histidine is His or H; Glutamine is Gln or Q; Asparagine is Asn or N; Lysine is Lys or K; Aspartic Acid is Asp or D; Glutamic Acid is Glu or E; Cysteine is Cys or C; Tryptophan is Trp or W; Arginine is Arg or R; and Glycine is Gly or G. For further description of amino acids, please refer to Proteins: Structure and Molecular Properties by Creighton, T.E., W.H. Freeman & Co., New York 1983.

The term "positively charged amino acid" refers to any amino acid having a positively charged side chain under normal physiological conditions. Examples of positively charged amino acids are Arg, Lys and His. The term "negatively charged amino acid" refers to any amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged amino acids are Asp and Glu. The term "hydrophobic amino acid" refers to any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of hydrophobic amino acids are Ala, Leu, Ile, Gly, Val, Pro, Phe, Trp and Met. The term "hydrophilic amino acid" refers to any amino acid having an uncharged, polar side chain that is

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relatively soluble in water. Examples of hydrophilic amino acids are Ser, Thr, Tyr, Asp, Gln, and Cys. "aromatic amino acid" refers to any amino acid comprising a ring structure. Examples of aromatic amino acids are His, Phe, Trp and Tyr.

term "charge relay system" refers to a His-Asp arrangement as described by Fersht & Sperling, 1973, J. Mol. Biol. 74:137-149; Blow et al., 1969, Nature 221:337-340.

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information obtained from the three-dimensional structures of the present invention reveal that HDLP has a single-domain structure that belongs to the open α/β class of folds (see, e.g., Branden, 1980, Q. Rev. Biophys. 13:317-38). Two orthogonal views of the overall three-15 dimensional structure of HDLP are depicted in Figure 4A and The HDLP structure has a central eight-stranded 4B. parallel β sheet (strands arranged as $\beta 2 \text{-}\beta 1 \text{-}\beta 3 \text{-}\beta 8 \text{-}\beta 7 \text{-}\beta 4 \text{-}\beta 5 \text{-}$ $\beta6)$, and sixteen α helices (labeled $\alpha1$ through $\alpha16$ respectively). See Figure 4C. Four of the helices pack on 20 either face of the β sheet (α 7, α 8, α 9, α 10 and α 11, α 12, α 13, α 14) forming the core α/β structure characteristic of this class of folds. Most of the remaining eight helices are positioned near one side of the β sheet, near stands $\beta2\text{--}$ β 1- β 3- β 8. Large, well defined loops (Loops L1-L7; Figure 25 4C) originate from the C-terminal ends of the β -strands. The extra helices and the large L1-L7 loops are associated with a significant extension of the structure beyond the core α/β motif. This extension of the structure gives rise to two prominent architectural features: a deep, narrow 30 pocket and an internal cavity adjacent to the pocket. These

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two architectural features comprise the active site (see Figure 5A). The structure of HDLP-related proteins (e.g. HDACs) may also comprise the conserved α/β structure characteristic.

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The term "active site" comprises any or all of the following sites in HDLP, the substrate binding site, the site where the cleavage of an acetyl group from a substrate occurs or the site where an inhibitor of the HDAC family or, more particularly, HDLP binds. The active site, as referred to herein, comprises Aspl66, Asp258, His170, Tyr297, His131, His132, Asp168, Asp173, Phe141, Phe198, Leu265, Pro22 and Gly140, and also a metal bound at the bottom of the pocket by Asp173, Asp168 and His defined by the coordinates listed in Figures 16 to 19 with an rmsd of 2.0 Å. The metal which binds at the bottom of the pocket will be a divalent cation selected from the group consisting of zinc, cobalt or manganese.

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The deep narrow pocket has a tube-like shape with a depth of ~ 11 Å. The pocket opening constricts half way down to ~ 4.5 by 5.5 Å, and becomes wider at the bottom (see Figure 5A). The pocket and its immediate surroundings are made up of loops L1 through L7.

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The walls of the pocket are covered with side chains of hydrophobic and aromatic residues (Pro22, Tyr91 near the entrance; and Gly140, Phe141, Phe 198, Leu265 and Tyr297 further down; Figure 5B). For numbering of amino acids please refer to SEQ ID NO:1. Of particular interest are Phe141 and Phe198, whose phenyl groups face each other in

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parallel at a distance of 7.5 Å, marking the most slender portion of the pocket (see Figure 5B). Of particular interest is that only one pocket residue differs in HDAC1 when the sequences are aligned (alignment may be accomplished using DNAstar™ MegAlign™ program, Madison, WI), this residue is Glu98 of HDAC1 which is Tyr91 in HDLP. The structure reveals that this residue in HDLP is mostly solvent exposed.

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Near the bottom of the pocket of the active site at its narrowest point, is located a zinc ion (see Figure 6A). In order to obtain the zinc in the structure, the crystals may be soaked in zinc (e.g. ZnCl₂) or co-crystalized in the presence of zinc. The zinc ion is coordinated by Aspl68 (Oδ1, 2.1 Å), His170 (Nδ1, 2.1 Å), Asp258 (Oδ1, 1.9 Å) and a water molecule (2.5 Å). See Figure 5B and 6B. The amino acid residues that coordinate zinc are arranged in a tetrahedral geometry, but the position of the water molecule, which is also hydrogen bonded to His131, deviates from this geometry by ~25°.

In addition to the zinc ligands, the bottom of the pocket contains two histidine (His131 and His132), two aspartic acids (Asp166 and Asp173) and a tyrosine (Tyr297). See Figure 5B and 10B. Each of the histidines makes a hydrogen bond through its N δ 1 to an aspartic acid carboxylate oxygen, with the oxygen located in the plane of the imidizole ring (Figure 5B). This His-Asp arrangement is characteristic of the charge relay system present in the active sites of serine proteases, where it serves to polarize the imidizole Ne and increase its basicity. Fersht & Sperling, 1973, J.

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Mol. Biol. <u>74</u>:137-149; Blow et al., 1969, Nature <u>221</u>:337-340.

The Asp166-His131 charge pair relay (hereafter referred to as "buried charged relay") is positioned even deeper in the pocket and more buried compared to the Asp173-His132 charge relay (hereafter referred to as "exposed charge relay") which is partially solvent exposed. The buried charge relay makes a hydrogen bond (2.6 Å) to the zinc-bound water molecule referred to above, and this hydrogen bond could contribute to the deviation of the water-zinc coordination from ideal geometry (Figure 5B). The exposed charge relay is directed to a point ~ 2.5 Å away from the water molecule and closer to the surface.

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Tyr 297 is positioned next to the zinc, opposite from where the two charge relay systems are located. The Tyr hydroxyl group lies 4.4 Å away from the zinc atom and has no interactions with the rest of the protein (Figure 5B). Next to Tyr297, there is an opening in the pocket wall, which leads to the adjacent internal cavity.

The floor of the internal cavity is made up of portions of the L3 and L7 loops as they emerge from the β strands, and the roof is made up by the $\alpha 1\text{-L} 1\text{-}\alpha 2$ segment. The L1 loop appears more flexible than other loops in the structure. This may allow the transient exchange of the cavity contents with the bulk solvent.

The cavity is lined primarily with hydrophobic residues and is particularly rich in glycine residues (Ala127, Gly128, Gly129, Met130, and Phe141 of L3; Gly293, Gly294, Gly295 and

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Gly296 of L7; and Tyr17, Pro22 and Leu23 of L1). There are only two charged residues in the cavity (Arg27 and His 21) and these are contributed by the L1 loop.

The cavity may provide space for the diffusion of the acetate product away from the catalytic center, which may otherwise be crowded and shielded during deacetylation from the solvent when the substrate is bound. Such a role for the cavity is supported by the observation that the cavity contains three water and two isopropanol molecules (from the crystallization buffer) in the 1.8 Å apo-protein structure. The cavity may also bind another cofactor, in addition to zinc, for the facilitation of the enzymatic activity of the HDLP. A proposed catalytic mechanism for deacetylation is provided in Figure 8.

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The structure of HDLP as defined by the present invention, in conjunction with the HDAC1 sequence homology, shows that the 375-amino acid HDLP protein corresponds to the histone deacetylase catalytic core which is conserved across the HDAC family (see Figure 2). The 35.2% HDLP-HDAC1 sequence identity predicts structural similarity with a rmsd in $\mbox{\it C}\alpha$ positions of ~ 1.5 Å. Chothia and Lesk describe the relation between the divergence of sequence and structure of proteins in Embo J. 5:823-826 (1986). residue C-terminus of HDLP is likely to have a divergent structure since this region has lower homology to HDAC1, although the α 16 helix in this region is part of the conserved open α/β core fold and HDAC1 is likely to comprise a similar helix. However divergent this C-terminal region may be, this region is outside the active site and is likely to not effect the structure of the active site. Beyond the

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C-terminus of the histone deacetylase catalytic core, HDAC family members are divergent in length and sequence. In the HDAC family, this region (amino acid residues ~390-482) is highly polar, populated with acidic residues, and is likely to be flexible or loosely folded.

The HDLP-HDAC homology maps primarily to the hydrophobic core and to the L1-L7 loops, with portions of the loops that make up the pocket and adjacent cavity having the highest level of amino acid residue sequence conservation (Figure 9A Specifically, all of the polar residues in the and 9B). active site (the zinc ligands, the two charge relay systems, and Tyr297) and the hydrophobic residues that make up the walls of the pocket (Gly140, Phe141, Phe198 and Leu265) are identical. Among the residues that make up the internal cavity, the ones closest to the active site are either identical or conservatively substituted (for example, Leu23 \rightarrow Met and Met130 \rightarrow Leu). Surface residues around the pocket are conserved to a lesser extent, but are still above 35% average sequence identity.

The information obtained from the inhibitor-bound HDLP complex crystal structures of the present invention reveal detailed information which is useful in the design, isolation, screening and determination of potential inhibitor compounds which may inhibit HDLP/HDAC family members. As described above, the HDLP structure consists of a parallel β sheet with α helices packing against both faces (Figure 4A, 4B, and 4C). At one end of the β sheet, 7 loops (L1-L7) form a narrow, tube-like pocket which are lined with hydrophobic residues and which comprise a zinc binding site, several polar side chains, including two Asp-His charge

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relay systems. Mutation of the zinc ligands and other polar residues at the pocket bottom reduces or eliminates the catalytic activity.

The present inventors found that mutation at the Tyr297Phe site reduced activity. See also, Hassig et al., 1998, Proc. Natl. Acad. Sci. USA 95:3519-3524; Kadosh & Struhl, 1998, Genes Dev. 12:797-805. The elimination of activity by mutation of these residues indicates that this region is the enzyme active site. Adjacent to the active site, there is an internal cavity that may provide space for the diffusion of the acetate reaction product. Homology at the active site between HDLP and HDAC1, as described above, indicates that they share structural and functional homology.

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The inhibitor compound, trichostatin A (TSA) (Tsuji et al., 1976, J. Antibiotics 29:1-6) binds HDLP by inserting its long aliphatic chain, which has a hydroxamic acid group at one end, into the pocket (Figure 6A, 6B and 6C). The aliphatic chain makes multiple contacts in the well-like, hydrophobic portion of the pocket. The hydroxamic acid reaches the polar bottom of the pocket, where it coordinates the zinc in a bidentate fashion and also forms hydrogen bonds with the polar residues in the active site, including the two charge relay system histidines. The aromatic dimethylamino-phenyl group at the other end of the TSA chain makes contacts at the pocket entrance and serves to cap it. The amino acid residues of HDLP which contact TSA are conserved in HDAC, indicating that TSA binds and inhibits HDAC in a similar fashion to HDLP.

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In the complex, the hydroxamic acid, most of the aliphatic chain and part of the dimethylamino-phenyl group of TSA are buried (60% of TSA's surface area; Figure 6A). The hydroxamic acid group binds the zinc in a bidentite fashion forming bonds through its carbonyl (2.4 Å) and hydroxyl groups (2.2 Å) resulting in a penta-coordinated Zn²+ (Figure 6B and 6C). The hydroxamic acid hydroxyl group replaces the water molecule that binds to the zinc in the apo-HDLP structure described above. The hydroxamic acid also hydrogen bonds with both charge relay system histidines (hydroxyl oxygen to Hisl3l Ne2, 2.8 Å; and nitrogen to Hisl32 Ne2, 2.8 Å), and the Tyr297 hydroxyl group (2.4 Å; Figure 6B and 6C).

15 The 5-carbon long branched alkene chain of TSA fits snugly in the narrow portion of the pocket making multiple van der Waals contacts with all of the hydrophobic groups lining the pocket (Figure 6B and 6C). Near its center, the chain contains a methyl substituted carbon-carbon double bond 20 which is sandwiched between the phenyl groups of the Phe141 and Phe98 at the tightest point of the pocket (Figure 6A and The length of the alkene chain appears optimal for spanning the length of the pocket, and allowing contacts both at the bottom and at the entrance of the pocket, although, the cap group of Formula (I) may provide length to 25 span the pocket allowing for a shorter alkene chain (aliphatic chain).

At the entrance of the pocket, one face of the planar structure formed by the dimethylamino-phenyl and adjacent carbonyl groups of TSA makes contacts at the rim of the pocket (Pro22, Tyr91, Phe141; Figure 6B and 6C). This

packing is facilitated by the roughly 110° angle in the overall structure of TSA at the junction of the aliphatic chain and the dimethylamino-phenyl group (occurring at the sp³ hybridized C8 carbon). Upon TSA binding, the side chain of Tyr91, which is mostly solvent exposed, changes conformation to make space for the dimethylamino-phenyl group. This is the only change near the active site observed upon TSA binding.

The hydroxamic acid group is a common motif in zinc 10 metalloprotease inhibitors. See U.S. Patent No. 5,919,940 and 5,917,090; See also, Grams et al., 1995, Biochemistry 34:14012-14020; Lovejoy et al., 1999, Nat. Struct. Biol. 6:217-221; and Holmes & Matthews, 1981, Biochemistry 20:6912-6920. Like TSA, these inhibitors also coordinate 15 the active site zinc in a bidentate fashion using their hydroxamate hyroxyl and carbonyl oxygens, replace the nucleophilic water molecule with their hydroxamate hydroxyl groups and form hydrogen bonds to the general base (Grams et al., 1995, Biochemistry 34:14012-14020; Lovejoy et al., 20 1999, Nat. Struct. Biol. 6:217-221; and Holmes & Matthews, 1981, Biochemistry 20:6912-6920).

SAHA, which has a ~30-fold weaker inhibitory activity than

TSA (Richon et al., 1998, Proc. Natl. Acad. Sci. USA

95:3003-3007), binds HDLP similarly to TSA (see, e.g.,

Figure 4D). The SAHA hydroxamic acid group makes the same

contacts to the zinc and active site residues, and the

importance of these interactions is underscored by the loss

of activity of SAHA derivatives lacking the hydroxamic group

(Richon et al., 1998, Proc. Natl. Acad. Sci. USA 95:3003-

3007). The six-carbon long aliphatic chain of SAHA packs in the tube-like hydrophobic portion of the pocket. Compared to TSA however, SAHA's aliphatic chain packs less snugly and makes fewer van der waals contacts, in part, because SAHA lacks TSA's C15 methyl group branch. SAHA also lacks TSA's double bonds in this region, and this may lead to increased flexibility of the aliphatic chain. The cap group of SAHA consists of a phenyl-amino ketone group. In the crystal structure, the phenyl group has weak electron density, suggesting that it does not pack as well as the cap group of TSA. This may be due to the larger separation between the hydroxamic and cap groups of SAHA compared to TSA (compare TSA, Formula (II) and SAHA, Formula (III), below).

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25 (III)

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The determination of the structure of HDLP and HDLP bound to an inhibitory compound has enabled, for the first time, the identification of the active site of HDLP and of related HDLP proteins, such as proteins belonging to the HDAC family.

The three-dimensional structural information and the atomic coordinates associated with said structural information of HDLP bound to an inhibitory compound is useful in rational drug design providing for a method of identifying inhibitory compounds which bind to and inhibit the enzymatic activity of HDLP, HDAC family proteins and other histone deacetylaselike proteins related to HDLP. Said method for identifying said potential inhibitor for an enzyme comprising deacetylase activity comprises the steps of (a) using a three-dimensional structure of HDLP as defined by its atomic coordinates listed in Figure 16 to 19; (b) employing said three-dimensional structure to design or select said inhibitor; (c) synthesizing said potential potential inhibitor; (d) contacting said potential inhibitor with said enzyme in the presence of an acetylated substrate; and (e) determining the ability of said inhibitor to inhibit said deacetylase activity.

The potential HDLP and HDLP-related (e.g. HDAC) inhibitors identified by the method of the present invention are represented by formula (I)

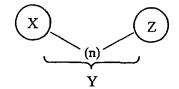
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(I)



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wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of proline and leucine; Y comprises an aliphatic chain group which binds to at least one amino acid selected from the group consisting of leucine, phenylalanine and glycine; and Z comprises an active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and wherein Z may further bind to a zinc atom and with the provision that the compound of Formula (I) is not TSA, trapoxin, SAHA, SAHA derivatives described in U.S. Patent Nos. 5,608,108; 5,700,811; 5,773,474; 5840,960 and 5,668,179.

The present invention permits the use of molecular design 20 techniques to design, identify and synthesize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site of HDLP and HDLPrelated proteins. The atomic coordinates of apo-HDLP and inhibitor-bound HDLP may be used in conjunction with 25 computer modeling using a docking program such as GRAM, DOCK, HOOK or AUTODOCK (Dunbrack et al., 1997, Folding & Design 2:27-42) to identify potential inhibitors of HDLP and ${\tt HDLP-related}$ proteins (e.g. ${\tt HDAC1}$). This procedure can 30 include computer fitting of potential inhibitors to the active site of HDLP to ascertain how well the shape and the

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chemical structure of the potential inhibitor will complement the active site or to compare the potential inhibitors with the binding of TSA or SAHA in the active See Bugg et al, 1998, Scientific American December:92-98; West et al., 1995, TIPS <u>16</u>:67-74. The potential inhibitors designed by modeling with a docking program conform to the general formula (I) as described Computer programs may also be employed to estimate above. the attraction, repulsion and stearic hindrance of the HDLP and potential inhibitor compound. Generally, the tighter the fit, the lower the stearic hindrances, the greater the attractive forces, and the greater the specificity which are important features for a specific inhibitory compound which is more likely to interact with HDLP and HDLP-related proteins rather than other classes of proteins. features are desired particularly where the inhibitory compound is a potential antitumor drug.

The compounds of the present invention may also be designed by visually inspecting the three-dimensional structure to 20 determine more effective deacetylase inhibitors. This type of modeling may be referred to as "manual" drug design. Manual drug design may employ visual inspection and analysis using a graphics visualization program such as "0" (Jones, T.A., Zhou, J.Y., Cowan, S.W., and Kjeldgaard, M., Improved 25 method for building protein models in electron density maps location of errors in and the these models, Acta Crystallog., A47, 110-119.

Initially potential inhibitor compounds can be selected for their structural similarity to the X, Y and Z constituents

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of formula (I) by manual drug design. The structural analog thus designed can then be modified by computer modeling programs to better define the most likely effective candidates. Reduction of the number of potential candidates is useful as it may not be possible to synthesize and screen a countless number of variations compounds that may have some similarity to known inhibitory molecules. analysis has been shown effective in the development of HIV protease inhibitors (Lam et al., 1994, Science 263:380-384; Wlodawer et al., 1993, Ann. Rev. Biochem. 62:543-585; Appelt, 1993 Perspectives in Drug Discovery and Design 1:23-48; Erickson, 1993, Perspectives in Drug Discovery and Design 1:109-128. Alternatively, random screening of an small molecule library could lead to potential inhibitors whose inhibitory activity may then be analyzed by computer modeling as described above to better determine their effectiveness as inhibitors.

The compounds designed using the information of the present invention may be competitive or noncompetitive inhibitors. These designed inhibitors may bind to all or a portion of the active site of HDLP and may be more potent, more specific, less toxic and more effective than known inhibitors for HDLP and HDLP-related proteins, particularly HDACs. The designed inhibitors may also be less potent but have a longer half life in vivo and/or in vitro and therefore be more effective at inhibiting histone deacetylase activity in vivo and/or in vivo for prolonged periods of time. Said designed inhibitors are useful to inhibit the histone deacetylase activity of HDLP and HDLPrelated proteins (e.g. HDAC1), to inhibit cell growth in

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vitro and in vivo and may be particularly useful as antitumor agents.

The present invention also permits the use of molecular design techniques to computationally screen small molecule data bases for chemical entities or compounds that can bind to HDLP in a manner analogous to the TSA and SAHA as defined by the structure of the present invention. computational screening may identify various groups which may be defined as "X", "Y" or "Z" of formula (I) above and may be employed to synthesize the potential inhibitors of the present invention comprising formula (I). potential inhibitors may be assayed for histone deacetylase inhibitory activity in a histone deacetylase activity assay (see Example 3 below), may be co-crystallized with HDLP to determine the binding characteristics through X-ray crystallography techniques defined above (e.g. said cocrystal structure may be determined by molecular replacement to assess the binding characteristics of said potential inhibitor), or may be assessed based on binding activity by incubating said potential inhibitor with said HDLP, performing gel filtration to separate any free potential inhibitor to HDLP-bound inhibitor, and determining the amount of histone deacetylase activity of the inhibitorbound HDLP. To measure binding constants (e.g., Kd), methods known to those in the art may be employed such as $\operatorname{Biacore}^{\operatorname{m}}$ analysis, isothermal titration calorimetry, Elisa with a known drug on the plate to show competitive binding, or by a deacetylase activity assay.

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The design of potential inhibitors of the present invention is further facilitated by reference to Figure 9, which is a surface representation figure that depicts the surface grooves. Analysis of such grooves gives insight into the constituents of the cap group of formula (I). The surface grooves are labeled groove A, groove A', groove B and groove C, into which additional cap groups may bind. The structure of HDLP bound to either TSA or SAHA shows that the cap groups of TSA and SAHA bind in groove A. By analysis of the amino acid sequence identity of HDLP and HDACs, Groove A is well conserved in HDACs, has a significant hydrophobic component, appears deep enough to allow for significant interactions and is also the largest of the four grooves. In addition to the dimethylamino phenyl group of the TSA, the A groove can fit approximately 200 daltons worth of groups (e.g. groove A could accommodate a naphthalene-like group after an appropriate spacer, etc.). Groove A. as referred to herein, is characterized by the following conserved residues of HDLP: His 21, Pro22, Lys24, Phe141, Leu265 and Phe335. The periphery of groove A comprises unconserved residues. Additionally, Groove A', as referred to herein, comprises primarily unconserved residues.

Groove B is immediately adjacent to the pocket. Of significance is that the bottom of groove B comprises the N-epsilon nitrogen of His170, which coordinates the zinc through its N-delta nitrogen. Significant binding energy may be achieved by contacting the Ne proton of His170 with a carboxylic acid or sulfate group. In addition, groove B may be large enough to fit a phenyl group, the face of which may comprise a partial negative charge which may pack over the N-epsilon proton of His170. The conserved residues of

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groove B, as referred to herein are: His170, Tyr196 and Leu265.

Groove C is not as well conserved as the other two grooves and the amino acid residues which comprise groove C are mostly polar and solvent exposed. Groove C, as referred to herein comprises the following conserved residues: Asn87, Gly140 and Phe198.

The compounds of the present invention are represented by formula (I):

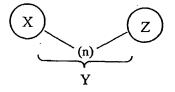
(I)

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Examples for suitable X constituents wherein X comprises a cap group may be described in three categories, depending upon which surface of groove A, A', B and/or C they are targeted to. The cap group may comprise all three categories on the same compound. Of particular benefit may be replacing the cap group of TSA or SAHA with a large, rigid structure. Nonlimiting examples for suitable cap groups (X) of formula (I) which may bind in groove A are: (1) attaching a 1-3 methyl linker followed by a phenyl or naphthalene group from the para or meta position of SAHA's phenyl group represented by formula (IV):

(IV)

$$n(H_2C)$$

- 45 **-**

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(2) attaching a 2-3 methyl linker followed by a phenyl or naphthalene group from the meta position of TSA's phenyl cap group, or from TSA's dimethyl amino group represented by formula (V):

(V)

phenyl or napthalene

phenyl or napthalene

n(H₂C)

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and which may bind in groove B is a 1-3 methyl group spacer followed by a carboxylate, sulfate or phenyl group as represented by formula (VI):

(VI)

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With respect to the aliphatic (Y) group, the diameter of the pocket suggests that one more methyl "side chain" could fit, in addition to the C15 methyl group on the C10 carbon. Nonlimiting suitable examples for Y constituents wherein Y comprises an aliphatic chain group are as follows: (1) add

a methyl group to TSA on the C12 carbon (with or without a methyl group on the C10 carbon and with or without double bonds and with or without substituting the X and/or Z constituents of formula (I)as represented by formula (VII): $\frac{1}{2}$

(VII)

10 (2) add a methyl group to TSA on the C9 carbon (with or without a methyl group on the C10 carbon; with or without both or either of the double bonds, and with or without substituting the X and/or Z constituents of formula (I) as represented by formula (VIII):

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(VIII)

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(3) replace the two alkalene double bonds of TSA with only one between C10 and C11, which may free the C11 and C12 torsion to allow for a better fit, the X and/or Z groups may also be substituted as represented by formula (IX):

25 (IX)

(X)

(4) cyclize C15 and C12 carbons of TSA through a sulphur atom (or nitrogen atom), the X and/or Z groups may also be substituted as represented by formula (X):

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(5) extend from the C9 carbon of TSA such that the extension approaches and/or enters groove B (see Figure 9); making C9 sp3 so that it can have some freedom; attach to C9 a 1-3 methyl group spacer which may include a double bond and they attaching thereto a sulfate, carboxylate, sulfate, hyroxyl, or phenyl group which may make an interaction with the N-epsilon proton of His170 which may coordinate the zinc atom as represented by formula (XI):

(XI)

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$$\begin{array}{c|c} X & \begin{pmatrix} 1_{15} \\ 1_{15}$$

25 (6) extend off the C8 carbon (replacing C14) of TSA such that the extension approaches or enters groove B; attach a 1-3 methyl group spacer (which may include a double bond) and then link thereto a carboxylate, sulfate, hydroxyl or phenyl group such that an interaction is made with the N-epsilon proton of His170 that coordinates the zinc atom; the X and/or Z constituents may also be substituted as represented by formula (XII):

(XII)

(7) substitute the C8 carbon at the end of the aliphatic chain such that the substitution may contact groove A, A', B and or C, in such an example, a cap group (X) may or may not be required and the X and Z constituents may be substituted as well, as represented by formula (XIII):

(XIII)

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$$X$$
 (1)
 (1)
 (2)
 (1)
 (3)
 (4)
 (4)
 (5)
 (7)
 (7)
 (8)
 (1)
 (8)
 (1)
 (8)
 (1)
 (8)
 (1)
 (8)
 (1)
 (8)
 (1)
 (8)
 (1)
 (1)
 (1)
 (2)

(8) formulas VII through XIII above wherein the aliphatic chain further comprises a methyl group between the active site binding group (Z) and the C8 carbon, and preferably just before the C8 carbon, increasing the distance between X and Z, (9) make the connection between the aliphatic chain and the cap group more rigid (e.g., by closing a 6-membered ring which may or may not comprise oxygen, the X and Z group may also be substituted as represented by formula (XIV):

(XIV)

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and (10) combining two or more of the changes depicted by formulas (VII-XIV).

Additionally, nonlimiting examples for suitable Z groups wherein Z comprises an active site binding group are as follows: (1) hydroxamic acid, (2) carboxylic acid, (3) sulfonamide, (4) acetamide, (5) epoxyketone, (6) an ester with a methyl linker and a hydroxyl of acetate ester group to lead into the cavity and interact with a conserved arginine (Arg27) as represented by formula (XV):

$$R_1$$
 CH_2 R_1 R_1 R_1 R_2 R_3 R_4 R_4 R_5 R_6 R_6

and (7) an alphaketone as represented by formula (XVI):
(XVI)

$$\begin{array}{c} \text{HQ} & \text{C} & \text{C} & \text{C} \\ \text{C} & \text{C} & \text{C} \\ \text{R}_1 & \text{C} & \text{C} & \text{C} \\ \text{C} \text{C} & \text{C} \\ \text{C} & \text{C} & \text{C} \\ \text{C} & \text{C} \\ \text{C} & \text{C} & \text{C} \\ \text{C} & \text{C} & \text{C} \\ \text{C} & \text{C} \\ \text{C} & \text{C} & \text{C} \\ \text{C} & \text{C} & \text{C} \\ \text{C} & \text{C} \\ \text{C} & \text{C} & \text{C} \\ \text{C} \\ \text{C} \\ \text{C} \\ \text{C} & \text{C} \\ \text{C} \\$$

Additionally, other suitable X, Y and Z constituents may be envisioned by the skilled artisan given the three-dimensional structural information of the present invention.

After having determined potential suitable X, Y and Z constituents, the constituents are combined to form a compound of formula (I) using combinatorial chemistry techniques. This may be achieved according to U.S. Patent Nos. 5,608,108; 5,700,811; 5,773,474; 5,840,960 and 5,668,179, incorporated herein by reference. Any methods

known to one of skill in the art may be employed to synthesize compounds of formula (I) comprising X, Y and Z constituents as determined by the methods described above.

- As mentioned above, the compounds of formula (I) are useful to inhibit the histone deacetylase activity of HDLP and HDAC-related proteins. Such inhibition may allow for a reduction or cessation of cell growth in vitro and in vivo.
- For in vitro use, such reduction or cessation of cell growth 10 is useful to study the role of histone deacetylation and differentiation during the cell cycle and also to study other mechanisms associated with cell cycle arrest and particularly how the repression of transcription is involved in cell cycle progression which may be studies in a yeast 15 model system such as that described by Kadosh & Struhl, 1998, Mol. Cell. Biol. <u>18</u>:5121-5127. In vitro model systems which may be employed to study the effects of potential inhibitors on cell cycle progression and also tumor growth include those described by: Richon et al, 1998, Proc. Natl. 20 Acad. Sci. USA 95:3003-3007; Yoshida et al., 1995, Bioessays 17:423-430; Kim et al., 1999, Oncogene 18:2461-2470; Richon et al., 1996, Proc. Natl. Acad. Sci. USA 93:5705-5708; and Yoshida et al., 1987, Cancer Res. 47:3688-3691.

For in vivo use, such a reduction or cessation of cell growth is useful to study the effect of said inhibitor compounds in non-human animal model systems of cancer and is also useful for the treatment of cancer in a recipient in need of such treatment. Non-limiting examples of animals which may serve as non-human animal model systems include

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mice, rats, rabbits, chickens, sheep, goats, cows, pigs, and non-human primates. See, e.g., Desai et al., 1999, Proc. AACR 40: abstract #2396; Cohen et al., 1999, Cancer Res., submitted. The compounds of the present invention may be administered to a transgenic non-human animal wherein said animal has developed cancer such as those animal models in which the animal has a propensity for developing cancer (e.g. animal model systems described in U.S. Patents 5,777,193, 5,811,634, 5,709,844, 5,698,764, and 5,550,316). Such animal model systems may allow for the determination of toxicity and tumor reduction effectiveness of the compounds of the present invention.

A preferred compound of the present invention may comprise high specific activity for HDLP and HDAC-related proteins, good bioavailability when administered orally, activity in reducing or ceasing cell growth in tumor cell lines, and activity in reducing or ceasing tumor growth in animal models of various cancers.

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Accordingly, another aspect of this invention is a method of eradicating or managing cancer in a recipient, which may be an animal and is preferably a human. Said method comprises administering to said recipient a tumor reducing amount of a compound as defined by formula (I) above, or a physiological acceptable salt thereof.

In a further aspect of the invention, there is provided a composition comprising the compound of formula (I) and an excipient or carrier. Administration of the foregoing agents may be local or systemic. Such carriers include any

suitable physiological solutions or dispersant or the like. The physiologic solutions include any acceptable solution or dispersion media, such as saline, or buffered saline. The carrier may also include antibacterial and antifungal agents, isotonic and absorption delaying agents, and the like. Except insofar as any conventional media, carrier or agent is incompatible with the active ingredient, its use in the compositions is contemplated.

- Routes of administration for the compositions containing the 10 delivery vehicle constructs of the present invention include any conventional and physiologically acceptable routes, such as, for example, oral, pulmonary, parenteral (intramuscular, intraperitoneal, intravenous (IV) or subcutaneous injection), inhalation (via a fine powder formulation or a 15 fine mist), transdermal, nasal, vaqinal, rectal, sublingual routes of administration and can be formulated in dosage forms appropriate for each route of administration.
- The following examples are provided to more clearly illustrate the aspects of the invention and are not intended to limit the scope of the invention.

EXAMPLES

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25 Example 1: Protein Production and Purification:

Full-length wild-type HDLP (Genbank accession number AE000719) was subcloned from an Aquifex aeolicus chromosomal DNA preparation (provided by Robert Huber of Universitaet of Regensburg, Germany) into the pGEX4T3 (Amersham-Pharmacia, Piscataway, NJ) vector using the polymerase chain reaction (PCR). The cysteine-to-serine and active site mutants were constructed by PCR site directed mutagenesis and were

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sequenced. The HDLP-glutathione S-transferase (GST) fusion protein was produced in Escherichia coli, purified by affinity chromatography using a column glutathione-sepharose resin (Amersham-Pharmacia, Piscataway, NJ), and by anion-exchange chromatography (Q-sepharose™; Amersham-Pharmacia, Piscataway, NJ). HDLP was cleaved from the fusion protein with thrombin at 4°C, was purified by anion-exchange (Q-sepharose™; Amersham-Pharmacia, Piscataway, (LN and gel filtration chromatography (Superdex[™]200; Amersham-Pharmacia, Piscataway, NJ), and was concentrated to typically 25 mg/ml in a buffer of 25 mM bis-tris propane (BTP), 500 mM NaCl, 5 mM dithiothrietiol (DTT), 2% isopropanol, pH 7.0.

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Although, it is not known what metal cofactor HDLP contains 15 in vivo, it is presumed to be zinc because of arrangement of the ligands and the similarities in the active site to the zinc proteases. The lack of metal in the purified HDLP is presumed due, in part, to the use of DTT 20 during purification. HDLP was reconstituted with Zn2+ by mixing the Cys75Ser/Cys77Ser double mutant at 10 mg/ml with a 5-fold molar excess of ZnCl₂ in a buffer of 25 mM bis-tris propane, 200 mM NaCl, 1% isopropanol, pH 7.0. Unbound ZnCl2 was removed by fractionating HDLP through a G25 desalting 25 column (Amersham-Pharmacia, Piscataway, NJ). The $\mbox{HDLP-Zn}^{2+}\mbox{-TSA}$ complex was prepared by incubating the \mbox{Zn}^{2+} reconstituted HDLP mutant with 1 mM TSA for 45 minutes, followed by gel filtration chromatography (Superdex™200; Amersham-Pharmacia, Piscataway, NJ) to remove excess TSA, and concentration to typically 25 mg/ml in a buffer of 25 mM 30 bis-tris propane, 500 mM NaCl, 1% isopropanol, pH 7.0.

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FLAG epitope tagged human HDAC1 was overexpressed using a baculovirus expression system in Hi5 (Invitrogen, Carlsbad, CA) insect cells grown in suspension in serum-free media (Sf900, Gibco, Grand Island, NY). The fusion protein was purified by anion exchange and affinity chromatography using Anti-FLAG M2 affinity resin (Sigma, St. Louis, MO) and FLAG Peptide (Sigma,, St. Louis, MO).

Example 2: Crystallization and data collection:

10 Crystals of apo-HDLP were grown at room temperature by the hanging-drop vapor-diffusion method, from 7.5% isopropanol, 28% PEG 1500, 425 mM NaCl, 100 mM Tris-Cl, pH 7.0. They form in space group C2 with a = 51.4 Å, b = 93.8 Å, c = 78.7 Å, β = 96.9 Å, and contain one HDLP molecule in the asymmetric unit. Diffraction data were collected with crystals flash-frozen in a buffer of 7.5% isopropanol, 35% PEG 1500, 75 mM NaCl, 100 mM Tris-Cl, pH 8.0, at -170° C.

The structure of the HDLP- $\rm Zn^{2+}$ complex was determined from HDLP Cys75Ser/Cys77Ser double mutant crystals grown from 23% tert-butanol, 27% PEG 1500, 400 mM KCl, 100 mM bis-tris propane-Cl, pH 6.8. Space group and cell dimensions were identical to the apocrystals. The HDLP- $\rm Zn^{2+}$ crystals were harvested and frozen in 27% tert-butanol, 22% PEG 1500, 50 mM KCl, 20 mM NaCl, 0.2 mM ZnCl₂, 100 mM bis-tris propane, pH 6.8, at -170° C.

Crystals of the HDLP-Zn²⁺-TSA complex comprised HDLP Cys75Ser/Cys77Ser double mutant and were grown from 23% tert-butanol, 27% PEG 1500, 600 mM KCl, 100 mM bis-tris propane-Cl, pH 6.8, by microseeding. The crystals were grown in the presence of zinc. They form in space group

 $P2_12_12_1$ with a = 53.4 Å, b = 94.4 Å, c = 156.3 Å and contain two HDLP- Zn^{2+} -TSA complexes in the asymmetric unit. The HDLP- Zn^{2+} -TSA crystals were harvested and frozen in the same cryobuffer as the HDLP- Zn^{2+} crystals except that 0.5mM TSA was added. Data were processed with DENZO and SCALEPACK (Otwinowski & Minor, 1997, Method. Ensemble. 276:307-326). MIR analysis, model building and refinement.

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The HDLP-Zn²⁺-SAHA complex crystals were grown and evaluated the same as the HDLP-Zn²⁺-TSA crystals. However, the restraints for the SAHA structure were constructed based on stereochemical parameters from TSA. Like the apo-HDLP crystals, the SAHA/HDLP co-crystals grew in space group C2.

Heavy-atom soaks were performed with the apo-HDLP crystals 15 in a buffer of 7.5% isopropanol, 30% PEG 1500, 75 mM NaCl, 100 mM Tris-Cl, pH 8.0, supplemented with 1.0 mM thimerosal for 2h, 5 mM KAu(CN)₂ for 1h, and 1 mM Pb(Me)₃OAc for 2h. MIR phases were calculated with the program MLPHARE (The 20 CCP4 suite: Programs for computational crystallography, 1994, Acta Crystallogr. D 50:760-763) at 2.5 Å using the anomalous diffraction signal from the thimerosal derivative, and had a mean figure of merit of 0.55. The phases were improved by solvent flattening with the program DM (The CCP4 25 suite: Programs for computational crystallography, 1994, Acta Crystallogr. D 50:760-763) , and were used to build the initial model with the program O (Jones et al., 1991, Acta Crystallogr. A 47:110-109). Successive rounds of rebuilding and simulated annealing refinement with the program CNS (Brunger et al., 1998, Acta Crystallogr. D 30 54:905-921) allowed interpretation of HDLP from residues 2

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to 373. Residues 1, 374, and 375 were not modeled and are presumed to be disordered.

The structure of the HDLP- $\mathrm{Zn^{2+}}$ -TSA and HDLP- $\mathrm{Zn^{2+}}$ -SAHA complex were determined by molecular replacement with the program 5 AMORE (The suite: Programs for computational CCP4 crystallography, 1994, Acta Crystallogr. D 50:760-763) using the apo-HDLP structure as a search model. The initial electron density maps had strong and continuous difference 10 density for the entire TSA molecule. However the SAHA molecule was not as well ordered in the cap group region. The structure of TSA was obtained from the Cambridge Structural Database (Refcode TRCHST) and was used to define stereochemical restraints used in the refinement with the program CNS. The restraints of SAHA were constructed based 15 on stereochemical parameters from TSA and surrounding amino acid residues. The dimer interface in the $HDLP-Zn^{2+}-TSA$ and $\mbox{HDLP-Zn}^{2+}\mbox{-SAHA}$ crystals primarily involves Phe200 on the The Phe200 side chain contacts Tyr91, protein surface. whose side chain conformation changes on TSA binding, and part of the dimethyl amino phenyl group of TSA from the second protomer. The HDAC family does not contain a phenylalanine residue at the equivalent position.

25 Example 3: Histone deacetylase assays:

Purified proteins were assayed by incubating 10 μg of [3H]acetyl-labeled murine erythroleukemia histone substrate and HDAC assay buffer (20 mM Tris-HCl, pH 8.0, 150 mM NaCl, 10% glycerol) for 30-60 minutes at 37° C in a total volume of 30 μ l. The final concentrations of HDLP and HDAC1-FLAG were 3.6 μ M and 0.24 μ M, respectively. Assays were performed in duplicate. The reactions were stopped and the

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released acetate was extracted and assayed as described (Hendzel et al., 1991, J. Biol. Chem. 266:21936-21942). [3H] acetyl-labeled murine erythroleukemia histones were prepared essentially as described (Carmen et al., 1996, J. Biol. Chem. 271:15837-15844). Inhibitors were added in the absence of substrate and incubated on ice for 20 minutes, substrate was added, and the assay performed as described above. HDLP was inclubated with 20 μ M ZnCl₂ and 20 μ M MnCl₂(H2O)₄ in HDAC buffer and tested for activity.

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Only HDLP dialyzed against ${\rm ZnCl_2}$ had activity. HDAC1-FLAG was dialyzed against 20 μM ${\rm ZnCl_2}$ in HDAC buffer which had no effect on activity. Therefore, HDAC1-FLAG contains a metal as purified.

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The *in vivo* substrate of HDLP is not known. HDLP may have a role in acetoin utilization like the *B. subtilis* AcuC gene product, and it has been annotated as such in the genome sequence, but the reaction catalyzed by AcuC is also not known. Furthermore, the *A. aeolicus* genome appears to lack the acuA and acuB genes that are part of the acuABC operon of B. subtilis (Deckert et al., 1998 Nature 392:353-358), and HDLP is as similar to human HDAC1 (35.2 % identity) as it is to B. subtilis AcuC (34.7 % identity).

What is claimed is:

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- A crystal of an enzyme comprising deacetylase activity 1. wherein said crystal effectively diffracts X-rays for 5 the determination of the atomic coordinates of said enzyme to a resolution of greater than 4 Å and wherein the structure of said enzyme comprises a conserved core α/β structure characteristic fold wherein said conserved α/β fold comprises an eight-stranded parallel β sheet and eight α helices and wherein four of the 10 helices pack on either face of said parallel β sheet and wherein said structure of said enzyme comprises an rmsd of less than or equal to 1.5 Å in the positions of $C\alpha$ atoms for at least 2/3 or more of the amino acids of HDLP as defined by the atomic coordinates of HDLP. 15
 - 2. The crystal of claim 1, wherein said protein structure further comprises:
 - (a) eight α helices positioned near one side of the β sheet; and
 - (b) at least seven large, well defined loops originating from the C-terminal ends of the β -strands of said eight-stranded parallel β sheet wherein the eight extra helices and the seven large loops are associated with a significant extension of the structure beyond the core α/β motif and wherein said extension of the structure gives rise to a deep, narrow pocket and an internal cavity adjacent to the pocket.

3. The crystal of claim 1, wherein said enzyme comprising deacetylase activity is selected from the group

consisting of HDLP, HDLP-related proteins, HDAC1, HDAC2, HDAC3, HDAC4, HDAC5, HDAC6, HDAC-related proteins, APAH, AcuC, and functional derivatives thereof.

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- 4. The crystal of claim 2 further comprising a specifically bound zinc atom in the active site of said enzyme.
- The crystal of claim 2 further comprising a specifically bound deacetylase inhibitor compound in the active site of said enzyme.
- 6. The crystal of claim 2 define by the atomic coordinates according to Figure 16.
- 7. A method for identifying a potential deacetylase inhibitor compound for an enzyme which comprises deacetylase activity, said method comprising the steps of:
 - a. using a three-dimensional structure of HDLP as defined by atomic coordinates according to Figure 16;
 - b. employing said three-dimensional structure to design or select said potential inhibitor;
 - c. synthesizing said potential inhibitor;
 - d. contacting said potential inhibitor with said enzyme in the presence of an acetylated substrate; and
- determining the deacetylase inhibitory activity of said potential inhibitor.

- 8. The method of claim 7, wherein the three-dimensional structure is designed or selected using computer modeling.
- 5 9. The method of claim 7, wherein the potential deacetylase inhibitor is designed de novo.
- 10. The method of claim 7, wherein the potential deacetylase inhibitor is designed based on a known inhibitor.
- 11. The method of claim 7, wherein said enzyme comprising deacetylase activity is selected from the group consisting of HDLP, HDLP-related proteins, HDAC1, HDAC2, HDAC3, HDAC4, HDAC5, HDAC6, HDAC-related proteins, APAH, and AcuC.
- 12. A method of evaluating the binding properties of the potential deacetylase inhibitor compound comprising the steps of:
 - a. co-crystallizing said compound with HDLP;

- b. determining the three-dimensional structure of said HDLP-potential inhibitor complex co-crystal by molecular replacement using the threedimensional structure of HDLP as defined by atomic coordinates according to Figure 16; and
- c. analyzing said three-dimensional structure of said HDLP bound to said potential inhibitor compound to evaluate the binding characteristics of said potential inhibitor compound.
- 13. A method for solving the structure of an HDAC family

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member crystal comprising the steps of:

- a. collecting X-ray diffraction data of said crystal wherein said data diffracts to a high resolution limit of greater than 4 Å;
- b. using the atomic coordinates of HDLP accoding to Figure 16 to perform molecular replacement or refinement and difference fourier with said X-ray diffraction data of said HDAC family member crystal to determine the structure of said HDAC family member; and
 - c. refining said structure of said HDAC family member.
- 14. The method of claim 13, wherein said HDAC family member is HDAC1.
 - 15. A Cys75Ser/Cys77Ser double mutant of HDLP wherein said mutant is encoded by the nucleic acid sequence of SEQ ID NO:4.
 - 16. A Cys75Ser/Cys77Ser double mutant of HDLP wherein said mutant has the amino acid sequence of SEQ ID NO:3.
 - 17. A nucleotide sequence according to SEQ ID NO:4
 - 18. An expression vector comprising the nucleotide sequence of claim 17.
- 19. A method of using the crystal of claim 1 for screening30 for a novel drug comprising:
 - a. selecting a potential ligand by performing

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rational drug design with the three-dimensional structure determined for the crystal;

- contacting the potential ligand with the ligand
 binding domain of the crystal; and
- c. detecting the binding potential of the potential ligand for the ligand binding domain, wherein the novel drug is selected based on its having a greater affinity for the ligand binding domain than that of a known drug.

Figure 1

Statistics from the crystallographic analysis

TABLE 1.

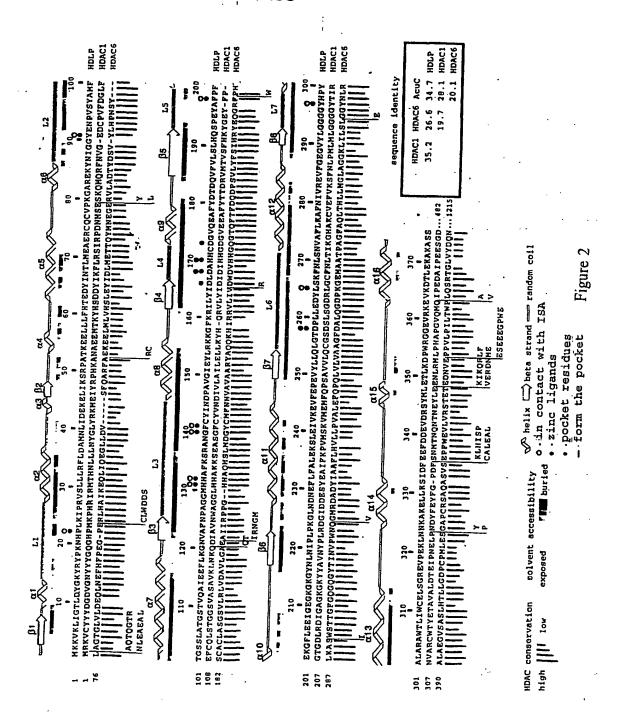
1/263

| | Data set | Na | Native th | thimerosal | Pb | AuCN | Zn | TSA | | |
|----------|---|---|---|--|---|---|---|--|--|--|
| SUBST | Space Group Resolution (A) Observations Unique reflections Data coverage (%) Rsym (%) | ," | C2 1.8 134,952 32,143 92.3 2.9 | C2 2.3 79,023 15,958 95.7 8.4 | C2 3.5 11,454 4,040 86.4 9.6 | C2 2.8 27,722 8,753 94.3 8.9 | C2 2.0 125,769 23,643 90.6 7.2 | P2,2,2, 2.1 180,427 50,796 93.8 7.1 | | |
| IIIIF 9 | phasing power Rcullis Rcullis (ano) | (| | 1.47 0.72 0.92 | 1.24 0.78 | 1.10 | SEE | | | |
| HFFT / | ment | | | · | | | • | RMSD | | |
| THIF 261 | Data Resolution Set (Å) HDLP HDLP-Zn 2.0 HDLP-Zn-TSA 2.1 | Reflections (IFI > 1σ) 31,550 23,582 44,122 | Total atoms 3214 3424 6475 | Water atoms 228 434 456 | H-factor (%) 19.8 22.0 | R-free (%) 24.0 25.8 | bonds (Å) 0.010 0.009 0.008 | angles (°) 1.63 1.48 1.78 | B-factor (Å ²) 3.55 1.04 3.83 | |

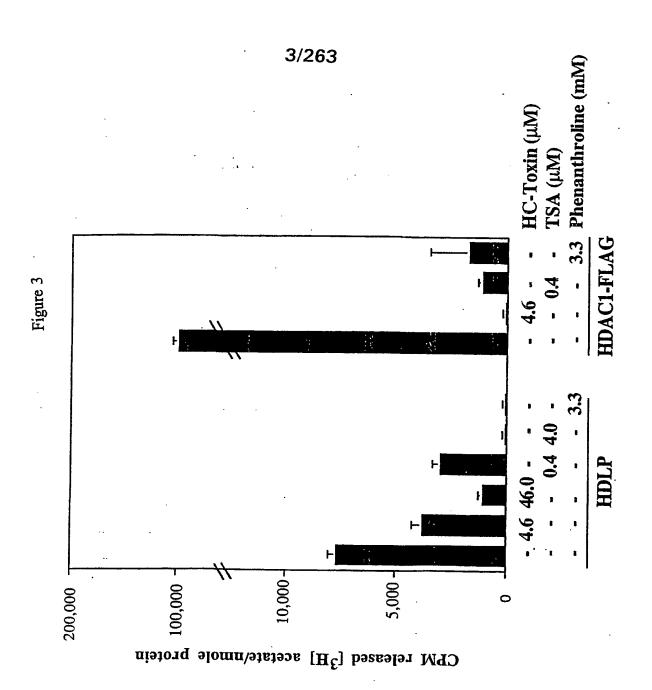
where <F $_{\lambda l}$ >is the root-mean-square heavy atom structure factor and E is the residual lack of closure error. Rcullis is the mean residual lack of closure error divided by the dispersive difference. R-factor = $\Sigma |F_{obs}$ omitted from the start of refinement. RMSD: root mean square deviations from ideal geometry and root $Rsym = \Sigma_h \Sigma_i \, \text{II}_{h,i} - c \text{I}_h \text{I}_h \text{I}_h \text{I}_h \text{I}_h \text{I}_h \text{I}_h \text{I}_h \text{II}_h \text{I$ $\mathsf{F}_{\mathsf{calc}}[l\Sigma|\mathsf{F}_{\mathsf{obs}}]$, where $\mathsf{F}_{\mathsf{obs}}$ and $\mathsf{F}_{\mathsf{calc}}$ are the observed and calculated structure factors, respectively. Figure of merit = IF(hkl)best//F(hkl). R-free = R-factor calculated using 5% of the reflection data chosen randomly and mean square variation in the B-factor of bonded atoms.

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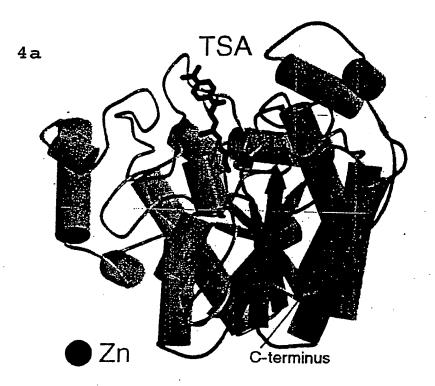


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4b

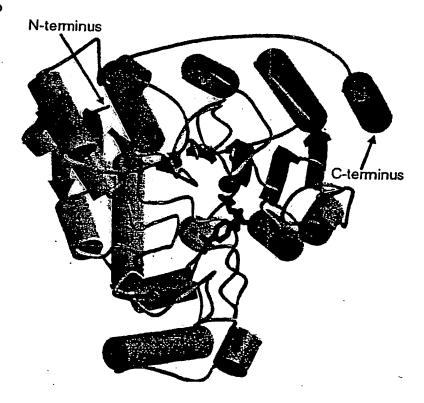


Figure 4
SUBSTITUTE SHEET (RULE 26)



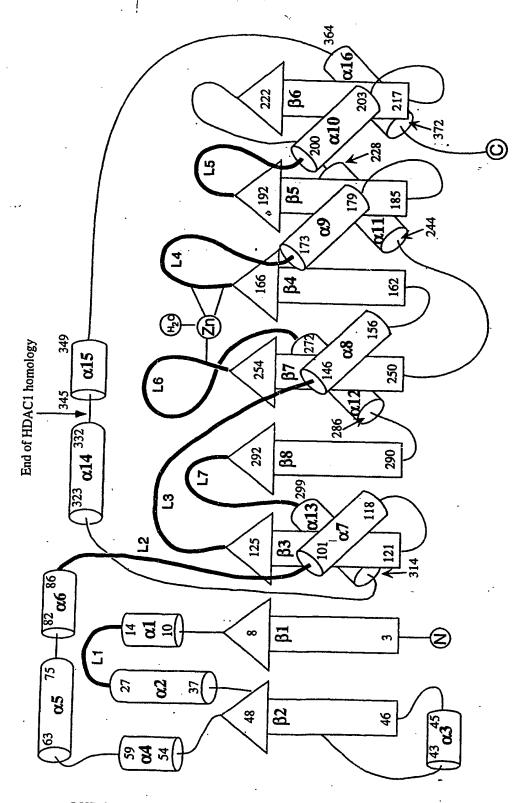


Figure 4c

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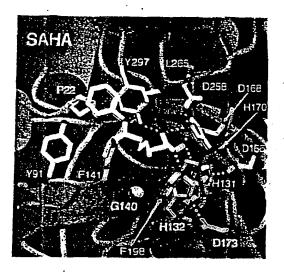
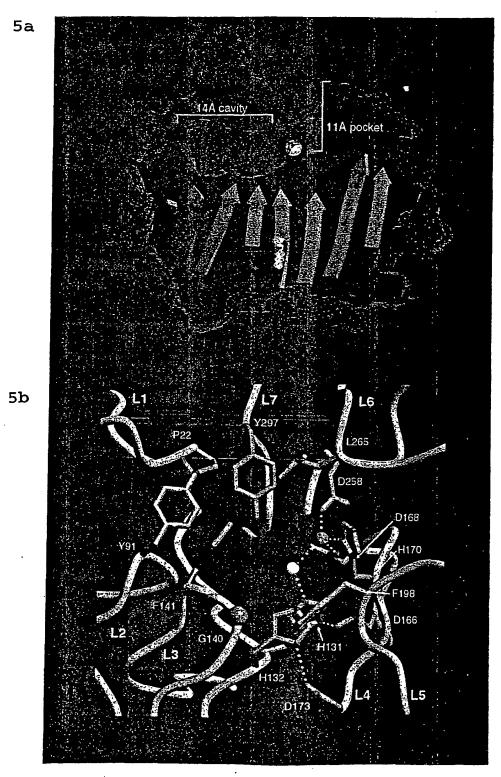


Figure 4D

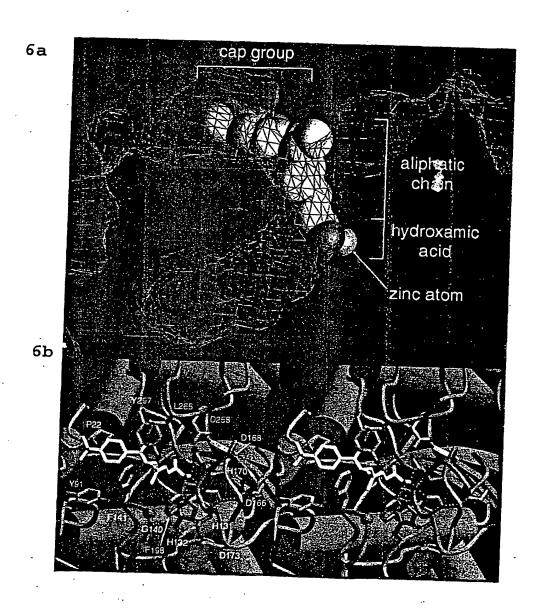
Figure 5 **7/263**



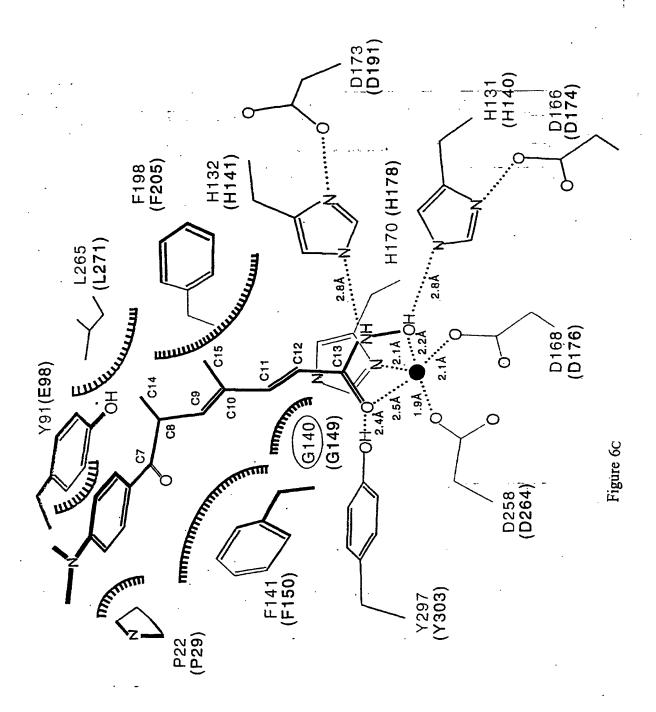
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Figure 6



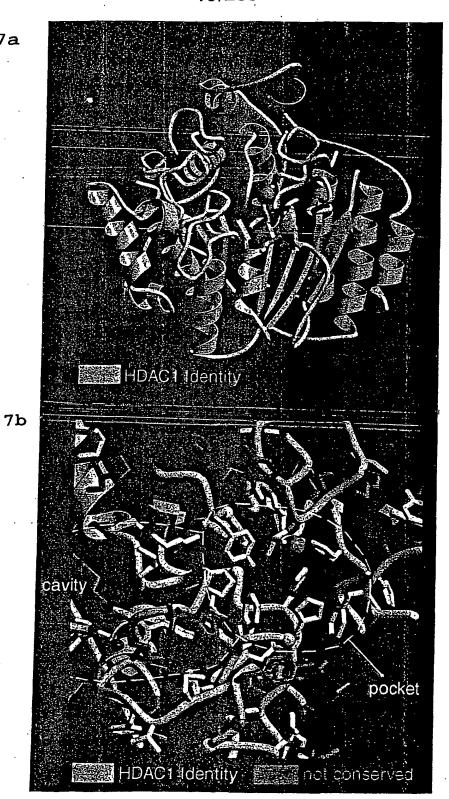
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Figure 7

7a



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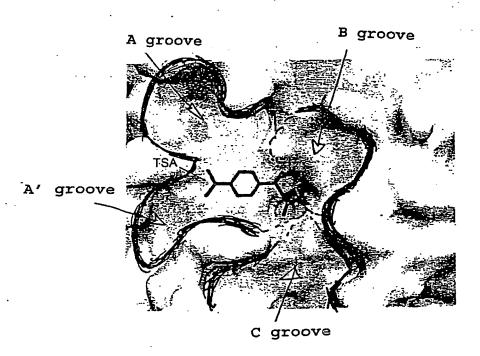


Figure 9

Figure 10

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10 20 30 40 ATGAAGAAGGITAAACTTATCGGAACTTTAGACTACGGAA 40 AGTACAGATATCCCAAAAACCATCCTCTTAAAATACCAAG 80 AGTTTCCCTACTCCTTAGGTTTTTAGATGCCATGAACCTT 120 ATAGATGAGAAGGAATTAATCAAGAGCAGACCCGCAACTA 160 AAGAAGAACTCCTTTTATTCCACACGGAAGACTACATAAA 200 210 220 230 240 CACTITAATGGAAGCGGAAAGGIGICAGIGCGIICCGAAG 240 GGAGCTAGGGAAAAGTACAACATAGGCGGATACGAAAACC 280 CCGTATCTTACGCGATGTTTACAGGCTCTTCTCTCGCAAC 320 GGGTTCAACAGTGCAGGCGATAGAGGAATTTTTTAAAGGGA 360 AATGTAGCTTICAATCCCGCGGGAGGTATGCACCACGCTT 400 410 420 430 440 TTAAAAGCAGGCAAACGCTTTTGCTACATAAACGACCC 440 CGCTGTGGGAATTGAGTACTTGAGAAAAAAAGGCTTTAAG 480 AGAATACTCTACATAGACCTTGATGCCCACCACTGCGACG 520 GIGITCAGGAAGCCITTIACGATACAGACCAGGIGITCGI 560 CCIGICCCITCACCAGICGCCGAGIACGCCITICCCITT 600 610 620 630 640 GAGAAGGCTTCCTGGAGGAGGAGGAAAAGGAA 640 AGGCTACAACCTGAACATTCCCCTGCCAAAGGCCTTGAA 680 CGACAACGAGTTCCTCTTTGCCCTAGAAAAATCTCTGGAA 720 ATAGTCAAAGAAGTATTTGAGCCCGAGGTTTACCTTCTTC 760 AACTCGGAACTGACCCACTCCTTGAAGATTACCTTTCCAA 800 810 820 830 840 1111 Lind and Lind an GTTCAACCTCTCAAACGTTGCCTTTTTTAAAAGCTTTCAAC 840 ATCGITCGTGAGGTTTTCGGGGAGGGAGTATACCTCGGAG 880 GAGGCGGATACCATCCTTACGCCCTCGCAAGGGCATGGAC 920 CCTAATCTGGTGCGAGCTTTCGGGAAGGGAAGTGCCGGAA 960 AAGCTAAACAATAAAGCAAAAGACTTTTAAAGAGTATAG 1000 1010 1020 1030 1040 ACTITGAAGAGTITGACGACGAGGTGGACCGCTCGTACAT 1040 GCTCGAAACCCTAAAGGACCCCTGGAGAGGAGGAGGGAGAGGTA 1080 AGGAAAGAAGTAAAGGATACGCTTGAAAAGGCGAAAGCCT 1120 CATCITA 1127

Figure 11

| 10 20 | 30 | 4 0 |
|--|--|--|
| <u> </u> | <u> </u> | Lil. |
| MKKVKLIGILDYGKYRYPKNHP | LKIPRVSLLLRFI | DAMNL 40 |
| IDEKELIKSRPATKEELLLFHI | EDYINTLMEAERO | COCALK 80 |
| GAREKYNIGGYENPVSYAMFIG | SSLATGSTVQATE | EFLKG 120 |
| NVAFNPAGGMHHAFKSRANGFC | YINDPAVGIEYLE | RKKGFK 160 |
| RILYIDLDAHHCDGVQEAFYDI | DQVFVL S LHQSPI | EYAFPF 200 |
| | | |
| 210 220 | 230 | 240 |
| | | |
| 210 220 | سيطسين | لسبل |
| EKGFLEEIGEGKGKGYNLNIPL | PKGI NINEFLFAI | EKSLE 240 |
| | | LIIIL LEKSLE 240 FLKAFN 280 |
| EKGFLFEIGEGKGKGYNLNIPL IVKEVFEPEVYLLQLGTDPLLE | .PKGLNDNEFLFAI DYLSKFNLSNVAI ARAWILIWCELSC | LEKSLE 240 FLKAFN 280 GREVPE 320 |

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Figure 12

| | 10 | 20 | 30 | 40 |
|----------|--|------------|--------------|-------------|
| بلبين | سلسيلين | بلبيبلت | بيلسييلي | علب |
| ATGAAG | AAGGITAAACT | TATCGGAACT | TTAGACTACG | GAA 40 |
| AGTACA | GATATCCCAAA | AACCATCCTC | TTAAAATACC | AAG 80 |
| AGTTTC | CCTACTCCTTA | GGTTTTTAGA | YTGCCATGAAC | CTT 120 |
| ATAGAT | GAGAAGGAATT | AATCAAGAGC | AGACCCGCAA | CTA 160 |
| AAGAAG | AACICCITTTA | TTCCACACGG | AAGACTACAT | AAA 200 |
| | 210 | 220 | 230 | 240 |
| بلبين | <u>,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,</u> | ىلىيىلى | يبلنسليب | لب |
| CACTITI | AATGGAAGCGG | AAAGGIGICA | GIGCGIICCG | AAG 240 |
| | AGGGAAAAGTA | | | |
| | CITACGCGAIG | | | |
| | AACAGTGCAGG | | | |
| AATGTA | CTTTCAATCC | CGCGGGAGGI | ATGCACCACG | CTT 400 |
| | 410 | 420 | 430 | 44 0 |
| عليين | <u></u> | | بالبيبان | <u> </u> |
| ΤΤΆλλλ | GCAGGGCAAAO | GGCTTTTGCT | 'ACAT'AAACGA | CCC 440 |
| | GGAATTGAGT | | | |
| AGAATAG | TCTACATAGA | CTTGATGCC | CACCACTGCG | ACG 520 |
| GIGITO | AGGAAGCCTTT | TACGATACAG | ACCAGGIGIT | CGT 560 |
| CCIGIC | CTTCACCAGI | CGCCCGAGTA | CCCTTICCC | |
| | 610 | 620 | 630 | 640 |
| | | | | |
| CACAAC | GCTTCCTGGA | | | • |
| | ACAACCTGAAC | | | |
| | CAGITICCTCT | | | |
| | AAAGAAGTATT | | · · | |
| | SAACTGACCCA | | | |
| FFICICO | | | | |
| _ | | 820 | 830 | 840 |
| | | | | <u> </u> |
| GIICAAC | CICICAAACGI | IGCCITITIZ | AAAGCITICA | AC 840 |
| ATCGTTC | FIGAGGITTIO | GGGGAGGGAG | TATACCTCGG | AG 880 |
| GAGGCGG | ATTCCATCCTT | ACGCCCTCGC | CAAGGGCATGG | AC 920 |
| CCTAATC. | PGGTGCGAGCT | ITCGGGAAGC | CAAGIGCCCC | AA 960 |
| AAGCTAA | ACAATAAAGCA | AAAGAGCTTT | TAAAGAGTAT | AG 1000 |
| | 1010 1 | .020 | 1030 | 1040 |
| ساسب | بريلينيلن | بيليبيا | سلسبل | |
| ACTTTGAZ | AGAGTTTGACG | ACGAGGIGGA | CCGCTCGTAC | AT 1040 |
| GCTCGAAA | ACCCTAAAGGA(| CCCTGGAGA | GGAGGAGAGG | TA 1080 |
| | AGTAAAGGATZ | | | |
| CATCITA | 4400 | | | |
| | 9 | ijuli gav | SHEET (M | ILL 26) |

Figure 13

| | 10 | 20 | 30 | 40 | • |
|-------------------------------|--------------------------------|--|------------------------|-------------------------------|-------------------|
| بيليني | <u> </u> | Lull | بيليييل | بلىسىل | |
| MKKVKLI | GILDYGK | YRYPKNHPLI | CIPRVSLLLF | FLDAMNL | 40 |
| IDEKELI | KSRPATK | <u>PELLILEHTE</u> | OYINI'LMEAE | RCQCVPK | 30 |
| GAREKYN | IGGYENP | VSYAMFTGSS | SLATGSTVQA | TEEFLKG | 120 |
| NVAFNPA | GGMHHAF | KSRANGFCY1 | NDPAVGIEY | LRKKGFK | 160 |
| RILYIDL | DAHHCDG | VQEAFYDIDÇ | OVFVLSLHQS | PEYAFPF | 200 |
| | | | | | |
| | 210 | 220 | 230 | 240 |) |
| | | | 230 | |) |
| | ستلب | سلسس | | لسبل | |
| EKGFLEE | IGEGKGK | EYNLNIPLPK | سلسنا | ALEKSLE | 240 |
| EKGFLEE | IGEGKGK(PEVYLLQI | GYNLNIPLPK GTDPLLEDY | GINDNEFLE | ALEKSLE AFLKAFN | 240 280 |
| EKGFLEE IVKEVFE IVREVFG | IGEGKGK PEVYLLQI EGVYLGO | GYNLNI PLPK GYDPLLEDY GGFHPYALAR | GLNDNEFLF LSKFNLSNV | ALEKSLE AFLKAFN SGREVPE | 240 280 320 |

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| 10 | 20 | 30 | 40 | |
|--------------|--------------------------|-------------|-----------------|------|
| - بايسىلىسىد | بالتبيلين | سلسسان | للسللب | |
| ATGAAGAAGGT | TAAACTTATCG | GAACTITAGA | CTACGGAA | 40 |
| AGTACAGATAT | CCAAAAAACCA | TCCTCTTAAA | ATACCAAG | 80 |
| AGITICCCTAC | ICCITAGGITI | TTAGATGCCA' | IGAACCIT | 120 |
| ATAGATGAGAA | GAATTAATCA | AGAGCAGACO | CGCAACTA | 160 |
| AAGAAGAACTC | TTTTATTCCA | CACGGAAGAC | TACATAAA | 200 |
| 210 | 220 | 230 | 240 |) |
| بليسليين | | سلسبان | لسياب | |
| CACTITAATGG | AAGCGGAAAGG | AGICAGAGCG | ITCCGAAG | 240. |
| GGAGCTAGGGA | AAAGTACAACA' | TAGGCGGATA | CGAAAACC | 280 |
| CCGTATCTTACC | CGATGITTAC | AGGCICTICI | CTCGCAAC | 320 |
| GGGTTCAACAG | rgcaggggata _l | GAGGAATTTT | TAAAGGGA | 360 |
| AATGTAGCTTTC | CAATCCCGCGG | GAGGTATGCA | CACGCTT | 400 |
| 410 | 420 | 430 | 44 0 |) |
| <u> </u> | سلسسلس | سلسسلب | لسسلس | |
| TTĄAĄĄGCAGGC | CAAACGGCTT | TTGCTACATA | AACGACCC | 440 |
| CGCTGTGGGAAT | TGAGTACTIG | AGAAAAAAAA | CTTTAA G | 480 |
| AGAATACICTAC | CATAGACCTIG | ATGCCCACCA | CTGCGACG | 520 |
| GIGITCAGGAAC | CCTTTTACGA | IACAGACCAG | SIGITCGI | 560 |
| CCTGTCCCTTCX | ACCAGICGCCC | GAGTACGCCT | ITCCCTTT | 600 |
| 610 | 620 | 630 | 640 |) |
| سلسسلس | بالبيلي | ببليبيلن | لسبليد | |
| GAGAAGGGCTTC | CIGGAGGAGA' | TAGGAGAAGG | AAAAGGAA | 640 |
| AGGGCTACAACC | TGAACATTCC | CCIGCCAAAG | GCTTGAA | 680 |
| CGACAACGAGIT | CCICITICCC | CTAGAAAAAI | CICIGGAA | 720 |
| ATAGTCAAAGAA | | | | 760 |
| AACICGGAACIC | ¿ACCCACTCCT | IGAAGAITAO | CTTTCCAA | 800 |
| 810 | 820 | 830 | . 840 |) |
| سلسسلسب | يطيبيلين | <u></u> | لسبيب | |
| GITCAACCICIC | 'AAACGI'IGCC | DAAAATTTTT | CTTTCAAC | 840 |
| ATOGITOGIGAG | CTTTTCGGGG | AGGGÄGTATA | CCTCGGAG | 880 |
| GAGGCGGATACC | 'ATCCTTACGC | CICGCAAGG | GCATGGAC | 920 |
| CCTAATCIGGIG | CGAGCTTTCGC | GAAGGGAAG | TGCCGGAA | 960 |
| AAGCTAAACAAT | 'AAAGCAAAAG | AGCTTTTAAA | GAGTATAG | 1000 |
| 1010 | 1020 | 1030 | 104 | 0 |
| سلسسلس | <u>سلىسىلىر</u> | سلسسا | 4 | |
| ACTTIGAAGAGI | TIGACGACGAC | GIGGACCGC | ICGIACAT | 1040 |
| GCICGAAACCCI | 'AAAGGACCCC | IGGAGAGGAG | GAGAGGTA | 1080 |
| AGGAAAGAAGTA | AAGGATACGC | MGAAAAGGO | GAAAGCCT | 1120 |
| CATCITA 1127 | | | | |

Figure 15

| | 10 | 20 | 30 | 40 | * |
|--------------------|----------------------------|---|------------------------------------|-------------------------------|------------|
| سلسب | ليتبلين | سسلنس | بتتليينا | بلىبىل | |
| MKKVKL | IGTLDYGKYI | RYPKNHPLK | IPRVSLLLR | FLDAMNL | 40 |
| IDEKEL | CKSRPATKE | ELLLFHTED | YINTLMEAE | RŞQSVPK | 80 |
| GAREKY | VIGGYENPV: | SYAMFTGSSI | LATGSTVQA | IEEFLKG | 120 |
| NVAFNP | AGGMHHAFK! | SRANGFCYII | VDPAVGIEY | LRKKGFK | 160 |
| RILYIDI | LDAHHCDGV | QEAFYDIDQ\ | VFVLSLHQS | PEYAFPF | 200 |
| | | | | | |
| • | 210 | 220 | 230 | 240 |) |
| بليتنا | 210 | 220 | 230 بىلىيىا | 240 ليتيل |) |
| EKGFLEI | 210 LILLIL EIGEGKGKG | سيليب | سلسا | للسيل |) 240 |
| | لينيلين | YNLNIPLPKO | SLNDNEFLF | ALEKSLE | |
| IVKEVFI | EIGEGKGKG | YNLNIPLPK(| ELNDNEFLF SKFNLSNV | aleksle aflkafn | 240 |
| IVKEVFI IVREVFO | EIGEGKGKG EPEVYLLQL | YNI NI PLPK STDPLLEDYI SYHPYALARA | GLNDNEFLF SKFNLSNV AWILIWCEL | ALEKSLE AFLKAFN SGREVPE | 240 280 |

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| Figure 16-1 | Fi | gure | 1 | 6-1 | |
|-------------|----|------|---|-----|--|
|-------------|----|------|---|-----|--|

| | | Residue # | X | Y | Z | OCC. B | |
|---------|---------------------|-----------|--------|--------|------------------|----------------------|-------------|
| | | | | 36.880 | 75.042 | OCC. B 1.00 59.90 | Segment ID: |
| ATCM : | 1 CB ALA 2 C ALA | | 45.336 | | 73.628 | 1.00 52.57 | AAAA : |
| | | | 46.410 | 38.631 | | | nana , |
| | 3 O ALA | | 45.780 | 39.595 | 74.052 | 1.00 62.46 | AAAA |
| | 4 N ALA | | 47.540 | 37.826 | 75.673 | 1.00 58.52 | AAAA |
| ATOM ! | 5 CA ALA | | 46.568 | 37.432 | 74.527 | 1.00 57.32 | AAAA : |
| ATOM | 6 N LYS | 3 | 46.890 | 38.570 | 72.389 | 1.00 39:51 | AAAA |
| STOM | 7 CA LYS | 3 | 46.687 | 39.669 | 71.440 | 1.00 29.58 | አጸጸአ |
| | 8 CE LYS | 3 | 47.855 | 39.763 | 70.459 | 1.00 35.03 | AAAA · |
| | 9 CG LYS | | 49.217 | 40.007 | 71.102 | 1.00 55.16 | AAAA |
| ATOM 1 | | | 50.315 | 40.000 | 73.039 | 1.00 65.28 | AAAA |
| ATOM 1 | | | 51.700 | 40.163 | 73.655 | 1.00 73.41 | AAAA |
| _ | | | 52.791 | 40.047 | 59.642 | 1.00 69.64 | AAAA |
| | | | 45.407 | 39.422 | 70.642 | 1.00 23.29 | |
| ATOM 1 | | | | | | | AAAA |
| -ATOM 1 | | | 44.984 | 38.282 | 70.487 | 1.00 27.41 | -AAAA |
| | 5 N VAI | | 44.814 | 40.498 | 70.138 | 1.00 25.18 | AAAA |
| | 6 CA VAI | | 43.585 | 40.418 | 69.349 | 1.D0 22.20 | АААА |
| | .7 CB VAI | | 42.501 | 41.365 | 59.887 | 1.00 31.46 | AAAA |
| ATOM 1 | 8 CG1 VAI | | 41.214 | 41.202 | 59.066 | 1.00 26.55 | AAAA |
| ATOM 1 | .9 CG2 VAI | 4 د | 42.244 | 41.080 | 71.348 | 1.00 34.98 | AAAA |
| ATOM 2 | O C VAI | ٤ 4 | 43.983 | 40.851 | 67.961 | 1.00 25.33 | AAAA |
| ATOM 2 | 1 0 VAI | . 4 | 44.557 | 41.927 | 57.778 | 1.00 21.19 | AAAA |
| | 2 N LYS | 5 5 | 43.554 | 40.023 | 56.978 | 1.00 21.32 | AAAA |
| | 3 CA LYS | | 44.052 | 40.291 | 55.607 | 1.00 20.10 | AAAA |
| | 4 CE LY | _ | 45.047 | 39.214 | 55.177 | 1.00 23.35 | AAAA |
| | 5 CG LY | | 46.301 | 39.092 | 55.049 | 1.00 23.75 | AAAA |
| | 6 CD LY | | 47.183 | 40.334 | £5.919 | 1.00 23.70 | AAAA |
| ATOM -2 | | | 48.510 | 40.151 | 55.669 | 1.00 24.34 | AAAA |
| | 8 NZ LY | | 49.351 | 41.387 | 66.585 | 1.00 22.04 | |
| | 9 C LY | | 42.914 | 40.294 | £4.596 | 1.00 20.27 | AAAA |
| | | | 41.949 | 39.535 | 54.728 | 1.00 18.48 | AAAA |
| | O O LY | | 43.071 | 41.111 | 53.564 | 1.00 19.28 | AAAA |
| | 1 N LE | | | | 52.483 | 1.00 20.68 | |
| | 2 CA LE | | 42.097 | 41.156 | | | AAAA |
| | 3 CB LE | | 41.571 | 42.574 | 52.291 | 1.00 23.51 | AAAA |
| | 4 CG LE | | 40.373 | 42.712 | 51.342 | 1.00 30.59 | AAAA |
| | 5 CD1 LE | | 40.079 | 44.192 | 51.153 | 1.00 29.90 | AAAA |
| | 6 CD2 LE | | 40.557 | 42.085 | 59.995 | 1.00 38.98 | AAAA |
| | 37 C LE | | 42.964 | 40.701 | 51.237 | 1.00 13.17 | AAAA |
| | 8 . Q LE | | 43.911 | 41.249 | 60.919 | 1.00 22.31 | AAAA |
| ATOM 3 | 39 N IL | | 42.359 | 39.689 | 60.538 | 1.00 19.15 | AAAA |
| ATOM 4 | 10 CA IL | | 43.945 | 39.199 | 59.338 | 1.00 13.38 | AAAA |
| ATOM 4 | 41 CE IL | | 42.922 | 37.674 | 59.191 | 1.00 19.05 | AAAA : |
| ATOM 4 | 12 CG2 TL | | 43.930 | 37.162 | 53.144 | 1.00 16.45 | AAAA |
| ATOM | :3 CG1 IL | | 43.253 | 37.007 | 60.521 | 1.00 22.91 | aaaa |
| ATOM | 44 CD1 IL | Ξ 7 | 43.296 | 35.543 | 60.450 | 1.00 34.99 | AAAA , |
| ATOM - | 15 C IL | E 7 | 42.396 | 39.850 | 58.125 | 1.00 17.95 | . AAAA |
| ATOM 4 | 46 0 IL | E 7 | 41.188 | 39.729 | 57.928 | 1.00 19.07 | áááá |
| | 17 N GL | Y 9 | 43.193 | 40.562 | E7.330 | 1.00 17.70 | AAAA |
| | 48 · CA GL | Y 9 | 42.523 | 41.193 | 55.148 | 1.00 13.11 | AAAA |
| | 49 C GL | | 43.640 | 41.857 | 55.243 | 1.00 20.91 | AAAA |
| • | 50 O GL | | 44.849 | 41.840 | 55.504 | 1.00 22.27 | AAAA |
| | SI N TH | _ | 43.134 | 42.428 | 54.155 | 1.00 23.99 | AAAA ' |
| | 52 CA TH | | 43.950 | 43.141 | 53.183 | 1.00 25.95 | AAAA |
| | 53 CE TH | | 44.739 | 42.195 | 52.263 | 1.00 25.80 | AAAA |
| | | | 45.321 | 42.962 | 51.199 | 1.00 26.56 | AAAA |
| | 64 CG1 TH | | 43.823 | 41.144 | 51.657 | 1.00 25.24 | 2222 |
| | 55 CG2 TH | | | | 52.294 | 1.00 23.04 | AAAA ! |
| | 56 C TH | | 43.025 | 43.957 | | 1.00 23.05 | AAAA |
| **** | 57 O TH | | 41.872 | 43.582 | 52.082 51.781 | 1.00 23.05 | AAAA |
| • | 58 N LE | | 43.517 | 45.079 | | | |
| | 59 CA LE | | 42.690 | 45.896 | 50.895 | 1.00 32.55 | AAAA |
| | 60 CB LE | | 43.256 | 47,319 | 50.761 | 1.00 28.09 | AAAA |
| ATOM | 61 CG LE | | 43.142 | 48.256 | 51.958 | 1.00 33.00 | AAAA |
| ATCM : | 62 CD1 LE | U 10 | 41.580 | 48.403 | 52.347 | 1.00 26.65 | AAAA |
| | 63 CD2 LE | U 10 | 43.938 | 47.744 | 53.126 | 1.00 41.33 | AAAA |
| | 64 C LE | | 42.566 | 45.261 | -9.512 | 1.00 32.68 | AAAA |
| | 55 O LE | :ບ 10 | 41.736 | 45.584 | 48.702 | 1.00 26.97 | AAAA |
| | 56 N AS | | 43.377 | 44.234 | ;9.25 6 | 1.00 25.75 | AAAA |

Figure 16-2

| MOTA | 67 | CA ASP | 11 | 43.36 | 7 43.543 | 1 47.970 | 1.00 35.74 | AAAA |
|--------------|----------------|------------------|----------|------------------|------------------|------------------|--------------------------|-----------------------|
| ATOM | 68 60 | CB ASP | 11 | 44.47 | | | | AAAA |
| MOTA MOTA | 69 70 | CG ASP | 11 11 | 45.850 | | | | AAAA |
| ATOM | 71 | OD2 ASP | 11 | 46.11(46.69(| | , | | AAAA |
| ATOM | 72 | C ASP | 11 | 42.034 | | | | AAAA |
| ATOM | 73 | O ASP | 11 | 41.748 | | | | AAAA |
| MOTA | 74 | N TYR | 12 | 41.220 | | | | AAAA AAAA |
| ATOM | 75 | CA TYR | 12 | 39.923 | | | | AAAA |
| MOTA | 76 | CB TYR | 12 | 39.119 | | | 1.00 29.35 | AAAA |
| ATOM ATOM | | CG TYR | 12 | 39.648 | | | | AAAA |
| ATOM | | CD1 TYR | 12 12 | 40.137 40.592 | | | | AAAA |
| ATOM | | CD2 TYR | 12 | 39.629 | | | | AAAA |
| ATOM | | CE2 TYR | 12 | 40.077 | | | | AAAA |
| ATOM | 82 | CZ TYR | 12 | 40.554 | | | 1.00 13.00 | AAAA AAAA |
| MOTA | | OH TYR | 12 | 40.964 | 37.456 | | 1.00 23.49 | AAAA |
| ATOM | | C TYR | 12 | 39.144 | | | 1.00 26.67 | AAAA |
| MOTA MOTA | | O TYR N GLY | 12 13 | 38.307 | | | 1.00 30.51 | AAAA |
| MOTA | | CA GLY | 13 | 39.441 38.767 | | | 1.00 30.22 | AAAA |
| MOTA | | C GLY | 13 | 38.911 | 45.009 | 46.675 45.177 | 1.00 25.13 1.00 27.31 | AAAA |
| MOTA | 89 (| GLY | 13 | 38.096 | 45.522 | 44.415 | 1.00 27.31 | AAAA AAAA |
| ATOM | | V LYS | 14 | 39.937 | 44.269 | 44.755 | 1.00 33.56 | AAAA |
| ATOM | | CA LYS | 14 | 40.176 | 44.005 | 43.337 | 1.00 39.81 | AAAA |
| MOTA MOTA | | CB LYS | 14 14 | 41.680 | 44.026 | 43.031 | 1.00 51.10 | AAAA |
| MOTA | | D LYS | 14 | 42.292 41.757 | 45.424 | 42.907 | 1.00 64.99 | AAAA |
| MOTA | | E LYS | 14 | 42.183 | 45.639 | 41.692 40.336 | 1.00 72.74 1.00 67.25 | AAAA |
| MOTA | | IZ LYS | 14 | 41.637 | | 40.045 | 1.00 70.06 | AAAA A A AA |
| MOTA | | LYS | 14 | 39.589 | 42.688 | 42.834 | 1.00 39.98 | AAAA |
| ATOM | 98 0 | | 14 | 39.746 | 42.350 | 41.658 | 1.00 46.99 | AAAA |
| ATOM ATOM | 99 N 100 C | I TYR A TYR | 15 15 | 38.927 | 41.944 | . 43.717 | 1.00 32.64 | AAAA |
| ATOM | _ | B TYR | 15 | 38.318 38.996 | 40.655 39.512 | 43.355 | 1.00 41.01 | AAAA |
| MOTA | | G TYR | 15 | 40.496 | 39.571 | 44.126 44.033 | 1.00 26.48 1.00 34.97 | AAAA AAAA |
| ATOM | | D1 TYR | 15 | 41.289 | 39.401 | 45.167 | 1.00 43.28 | AAAA |
| MOTA | | El TYR | 15 | 42.677 | 39.548 | 45.106 | 1.00 36.05 | AAAA |
| ATOM ATOM | | D2 TYR E2 TYR | 15 | 41.127 | 39.879 | 42.827 | 1.00 40.78 | AAAA |
| ATOM | 107 C | | 15 15 | 42.508 43.275 | 40.027 39.865 | 42.756 | 1.00 37.13 | AAAA |
| ATOM | 108 0 | | 15 | 44.644 | 40.044 | 43.899 43.844 | 1.00 36.87 1.00 35.40 | AAAA |
| ATOM | 109 C | | 15 | 36.838 | 40.705 | 43.714 | 1.00 38.62 | AAAA AAAA |
| ATOM | 110 0 | | 15 | 36.344 | 39.868 | 44.468 | 1.00 37.82 | AAAA |
| MOTA | 111 N | | 16 | 36.141 | 41.703 | 43.177 | 1.00 44.85 | AAAA |
| ATOM ATOM | 112 CF | | 16 | 34.716 | 41.890 | 43.431 | 1.00 45.75 | AAAA |
| ATOM | 114 CC | | 16 16 | 34.320 35.170 | 43.348 44.399 | 43.187 | 1.00 54.17 | AAAA |
| ATOM | 115 CI | | 16 | 34.920 | 44.506 | 43.875 45.369 | 1.00 66.77 1.00 72.39 | AAAA |
| ATOM | 116 NE | | 16 | 35.649 | 45.646 | 45.923 | 1.00 85.39 | AAAA AAAA |
| MOTA | 117 CZ | | 16 | 35.489 | 46.906 | 45.518 | 1.00 81.94 | AAAA |
| MOTA | 118 NH | 11 ARG | 16 | 34.624 | 47.197 | 44.554 | 1.00 80.19 | AAAA |
| ATOM ATOM | | 12 ARG | 16 | 36.205 | 47.878 | 46.069 | 1.00 85.46 | AAAA |
| ATOM | 120 C 121 O | ARG ARG | 16 16 | 33.915 34.400 | 41.029 | 42.460 | 1.00 43.50 | AAAA |
| ATOM | 122 N | TYR | 17 | 32.689 | 40.667 40.692 | 41.385 42.833 | 1.00 38.62 | AAAA |
| ATOM | 123 CA | | 17 | 31.850 | 39.923 | 41.930 | 1.00 32.68 1.00 37.55 | AAAA AAAA |
| atom | 124 . CB | | 17 | 30.662 | 39.306 | 42.672 | 1.00 41.05 | AAAA |
| ATOM | 125 CG | | 17 | 31.040 | 38.104 | 43.519 | 1.00 37.51 | AAAA |
| ATOM | | 1 TYR | 17 | 32.039 | 38.194 | 44.493 | 1.00 32.59 | AAAA |
| ATOM TOM | | 1 TYR | 17 | 32.383 30.393 | 37.095 | 45.277 | 1.00 29.32 | AAAA |
| ATOM ATOM | | 2 TYR 2 TYR | 17 17 | 30.393 | 36.875 35.772 | 43.346 44.122 | 1.00 31.46 | AAAA |
| ATOM | 130 CZ | | 17 | 31.721 | 35.772 | 45.088 | 1.00 28.64 1.00 27.14 | AAAA |
| MOTA | 131 ОН | | 17 | 32.044 | 34.807 | 45.881 | 1.00 27.14 | AAAA AAAA |
| MOTA | 132 C | TYR | 17 | 31.380 | 40.871 | 40.836 | 1.00 40.97 | AAAA |
| | | | | | | | = | |

| | | | - | | | | | |
|--------|---------|-------|------|----------|---------|---------|------------|------|
| ATCM | 133 0 | TYR | 17 | 31.435 | 42.097 | 40.984 | 1.00 29.58 | AAAA |
| ATOM | 134 N | PRO | . 18 | 30.904 | 40.321 | 39.722 | 1.00 41.02 | AAAA |
| | 135 CI | | 18 | 30.760 | 38.910 | 39.318 | 1.00 48.67 | |
| ATOM | | | | | | | 1.00 48.67 | AAAA |
| ATOM | 136 C | | 18 | 30.459 | 41.197 | 38.649 | 1.00 49.35 | AAAA |
| ATCM | 137 CI | B PRO | 18 | 30.321 | 40.228 | 37.481 | 1.00 59.04 | AAAA |
| ATCM | 138 C | | 18 | 29.756 | 39:017 | 38.179 | 1.00 54.15 | AAAA |
| | | | | | | | | |
| atom | 139 C | PRO | 18 | 29.178 | 41.982 | 38.864 | 1.00 54.97 | AAAA |
| ATOM | 140 O | PRO | 18 | 28.457 | 41.823 | 39.850 | 1.00 46.85 | AAAA |
| ATCM | 141 N | LYS | . 19 | 28.961 | 42.868 | 37.904 | 1.00 60.87 | AAAA |
| | 142 C | | 19 | 27.777 | 43.696 | 37.749 | 1.00 67.78 | AAAA |
| ATOM | | | | | | | | |
| ATOM | 143 CI | | 19 | - 27.155 | 43.278 | | 1.00 73.26 | AAAA |
| ATOM | 144 CC | 3 LYS | 19 | 26.971 | 41.752 | 36.414 | 1.00 77.87 | AAAA |
| MOTA | 145 CI | LYS | ¨ 19 | 26.276 | 41.166 | 35.209 | 1.00 81.01 | AAAA |
| ATOM | 146 CI | | 19 | 26.039 | 39.680 | 35.471 | 1.00 82.45 | AAAA |
| | | | | | | | | |
| MOTA | 147 N2 | | 19 | 25.417 | 38.959 | 34.331 | 1.00 83.11 | AAAA |
| MOTA | 148 C | LYS | 19 | 26.688 | 43.594 | 38.814- | 1.00 64.15 | AAAA |
| MOTA | 149 O | LYS | 19 | 26.810 | 44.047 | 39.949 | 1.00 65.73 | AAAA |
| ATOM | 150 N | ASN | 20 | 25.604 | 42.986 | | 1.00 59.78 | AAAA |
| | | | | | | | | |
| atom | 151 CA | | 20 | 24.353 | 42.703 | 39.025 | 1.00 59.91 | AAAA |
| MOTA | 152 CE | 3 asn | 20 | 23.516 | 41.844 | 38.077 | 1.00 68.08 | AAAA |
| ATOM | 153 CG | ASN | . 20 | 22.108 | 42.355 | 37.907 | 1.00 78.73 | AAAA |
| MOTA | 154 OI | 1 ASN | 20. | 21.894 | 43.498 | 37.496 | 1.00 78.67 | AAAA |
| | | | | 21.132 | 41.505 | | | |
| MOTA | | 2 ASN | 20 | | | 38.211 | 1.00 83.22 | AAAA |
| MOTA | 156 C | ASN | 20 | 24.474 | 41.977 | 40.361 | 1.00 53.35 | AAAA |
| MOTA | 157 O | ASN | 20 | 23.611 | 42.112 | 41.234 | 1.00 59.92 | AAAA |
| ATOM | 158 N | HIS | 21 | 25.543 | 41.206 | 40.511 | 1.00 44.23 | AAAA |
| | 159 CA | | 21 | 25.768 | 40.397 | | 1.00 28.15 | AAAA |
| ATCM | | | , | | | | | |
| MOTA | 160 CB | | 21, | 27.088 | 39.639 | 41.570 | 1.00 31.84 | AAAA |
| ATOM | 161 CG | HIS | . 21 | 27.155 | 38.411 | 42.418 | 1.00 34.79 | AAAA |
| ATOM T | 162 CD | 2 HIS | 21 | 27.344 | 38.259 | 43.752 | 1.00 25.03 | AAAA |
| ATOM | | 1 HIS | 21 | 26.929 | 37.148 | 41.917 | 1.00 34.81 | AAAA |
| | | | | | | | | |
| ATOM | | 1 HIS | 21 | 26.979 | 36.269 | 42.900 | 1.00 17.01 | AAAA |
| ATOM | | 2 HIS | 21 | 27.228 | 36.917 | 44.026 | 1.00 32.31 | АААА |
| ATOM | 166 C | HIS | 21 | . 25.763 | -41.135 | 43.051 | 1.00 29.37 | AAAA |
| ATOM | 167 O | HIS | 21 | 26.346 | 42.210 | 43.186 | 1.00 28.54 | AAAA |
| ATOM | 168 N | PRO | 22 | 25.093 | 40.565 | 44.066 | 1.00 29,14 | AAAA |
| | 169 CD | | 22 | 24.301 | 39.322 | 44.061 | 1.00 31.20 | AAAA |
| ATOM | | | | | | | | |
| ATOM | 170 CA | | 22 | 25.034 | 41.185 | 45.395 | 1.00 32.84 | AAAA |
| ATOM | 171 CB | PRO | 22 | 24.174 | 40.192 | 46.187 | 1.00 34.98 | AAAA |
| ATOM | 172 CG | PRO | 22 | 23.257 | 39.634 | 45.109 | 1.00 30.11 | AAAA |
| ATOM | 173 C | PRO | 22 | 26.411 | 41.415 | 46.044 | 1.00 34.37 | AAAA |
| | 174 0 | PRO | 22 | 26.554 | 42.272 | 46.916 | 1.00 29.17 | AAAA |
| ATOM | | | | | | | | |
| ATOM | 175 N | LEU | 23 | 27.415 | 40.644 | 45.629 | 1.00 29.22 | AAAA |
| ATOM | 176 CA | LEU | 23 | 28.765 | 40.781 | 46.181 | 1.00 26.49 | AAAA |
| ATOM | 177 CB | LEU | 23 | 29.414 | 39.397 | 46.332 | 1.00 22.30 | AAAA |
| ATOM | 178 CG | LEU | 23 | 28.703 | 38.527 | 47.380 | 1.00 21.04 | AAAA |
| | | | | | | | 1.00 19.35 | |
| atom | | 1 LEU | 23 | 29.307 | 37.113 | 47.410 | | AAAA |
| ATOM | | 2 LEU | 23 | 28.850 | 39.197 | 48.746 | 1.00 26.51 | AAAA |
| ATOM | 181 C | LEU | 23 | 29.661 | 41.718 | 45.361 | 1.00 25.81 | AAAA |
| ATOM | 182 0 | LEU | 23 | 30.893 | 41.693 | 45.477 | 1.00 28.45 | AAAA |
| | | LYS | 24 | 29.018 | | | 1.00 24.86 | AAAA |
| | | | | | | | | |
| ATOM | 184 CA | LYS | 24 | 29.696 | 43.552 | 43.723 | 1.00 27.35 | AAAA |
| ATOM | 185 CB | LYS | 24 | 28.662 | 44.244 | 42.830 | 1.00 28.57 | AAAA |
| ATOM | 186 CG | LYS | 24 | 29.118 | | 42.171 | 1.00 52.95 | AAAA |
| | 187 CD | LYS | 24 | 28.025 | 46.603 | 42.283 | 1.00 63.74 | AAAA |
| ATOM | | | | | | | | |
| ATOM | 188 CE | LYS | 24 | 26.688 | 46.138 | 41.706 | 1.00 66.09 | AAAA |
| ATOM | 189 NZ | LYS | 24 | 25.595 | 47.137 | 41.896 | 1.00 66.00 | AAAA |
| ATOM | 190 C | LYS | 24 | 30.332 | 44.592 | 44.676 | 1.00 29.52 | AAAA |
| ATOM | 191 0 | LYS | 24 | 31.412 | 45.123 | 44.420 | 1.00 30.67 | AAAA |
| | | | | 29.652 | | 45.779 | 1.00 26.90 | AAAA |
| ATOM | 192 N | ILE | 25 | | 44.879 | | | |
| ATOM | 193 CA | ILE | 25 | 30.151 | 45.865 | 46.738 | 1.00 25.02 | AAAA |
| ATOM | 194 CB | ILE | 25 | 29.105 | 46.177 | 47.824 | 1.00 28.34 | AAAA |
| ATOM | | : ILE | 25 | 27.961 | 46.951 | 47.237 | 1.00 23.84 | AAAA |
| | | ILE | 25 | 28.661 | 44.869 | 48.495 | 1.00 30.31 | AAAA |
| ATOM | 196 CG1 | | | | | | 1.00 44.90 | |
| ATOM | | ILE | 25 | 27.718 | 45.051 | 49.660 | | AAAA |
| ATOM | 198 C | İΙΕ | 25 | 31.424 | 45.463 | 47.483 | 1.00 32.19 | AAAA |
| | | | | | | - | | • |

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| | • • • • | _ | ~ | | | | | | |
|--------|---------|-----|-------|------------|--------|--------|--------|------------|--------|
| MOTA | 199 | | ILE | | 31.736 | 44.271 | | 1.00 26.54 | AAAA |
| ATOM | 200 | N | PRO | 26 | 32.191 | 46.463 | 47.956 | 1.00 30.14 | AAAA |
| ATOM | 201 | CI | PRO | 26 | 31.979 | 47.907 | 47.770 | 1.00 36.38 | AAAA |
| ATOM | 202 | | | | 33.431 | 46.241 | | 1.00 30,63 | |
| | | | | | | | | | AAAA |
| MOTA | 203 | | | | 34.014 | 47.652 | | 1.00 34.29 | AAAA |
| ATOM - | 204 | CG | PRO | 26 | 33.397 | 48.373 | | 1.00 43.39 | AAAA |
| MOTA | 205 | С | PRO | 26 | 32.943 | 45.727 | 50.061 | 1.00 25.99 | AAAA |
| ATOM | 206 | 0 | PRO | 26 | 31.854 | 46.110 | | 1.00 25.51 | • |
| | | | | | | | | | AAAA |
| MOTA | 207 | | ARG | | 33.719 | 44.880 | | 1.00 21.98 | AAAA |
| ATOM | 208 | | | 27 | 33.267 | 44.347 | 52.035 | 1.00 26.17 | AAAA |
| ATOM | 209 | CE | ARG | 27 | 32.641 | 42.969 | 51.834 | 1.00 22.70 | AAAA |
| ATOM | 210 | CG | ARG | . 27 | 31.442 | 43.039 | 50.890 | 1.00 26.75 | AAAA |
| MÔTA | 211 | CD | | 27 | 30.832 | 41.672 | 50.581 | | |
| | | | | | | | | | AAAA |
| ATOM | 212 | NE | | 27 | 30.121 | 41.098 | 51.716 | 1.00 28.66 | AAAA |
| ATOM | 213 | CZ | ARG | 27 | 30.582 | 40.129 | 52.503 | 1.00 31.79 | AAAA |
| ATOM | 214 | NH | 1 ARG | 27 | 31.778 | 39.598 | 52.290 | 1.00 34.08 | - AAAA |
| ATOM | 215 | | 2 ARG | 27 | 29.833 | 39.688 | 53.505 | 1.00 26.16 | |
| | | | ARG | 27 | | | | | AAAA |
| ATOM | 216 | C | | | 34.358 | 44.297 | 53.090 | 1.00 24.10 | AAAA |
| ATOM | 217 | 0 | ARG | 27 | 34.326 | 45.074 | 54.038 | 1.00 23.50 | AAAA |
| ATOM | 218 | N | VAL | 28 | 35.314 | 43.390 | 52.960 | 1.00 21.45 | AAAA |
| ATOM | 219 | CA | VAL | 28 | 36.385 | 43.385 | 53.953 | 1.00 21.75 | AAAA |
| ATOM | 220 | CB | VAL | 28 | 37.221 | 42.101 | 53.866 | 1.00 26.55 | |
| | | | | | | | | | AAAA |
| ATOM | 221 | | 1 VAL | 28 | 38.407 | 42.177 | 54.830 | 1.00 23.84 | AAAA |
| ATOM | 222 | CG | 2 VAL | 28 | 36.337 | 40.906 | 54.214 | 1.00 19.20 | AAAA |
| MOTA | 223 | С | VAL | 28 | 37.277 | 44.611 | 53.736 | 1.00 20.86 | AAAA |
| ATOM | 224 | 0 | VAL | 28 | 37.770 | 45.223 | 54.702 | 1.00 25.15 | AAAA |
| ATOM | 225 | N · | | 29 | 37.480 | 44.996 | 52.475 | 1.00 19.22 | |
| | | | | | | | | | AAAA |
| MOTA | 226 | CA | SER | . 29 | 38.320 | 46.169 | 52.209 | 1.00 19.63 | AAAA |
| MOTA | 227 | CB | SER | 29 | 38.591 | 46.352 | 50.702 | 1.00 24.45 | AAAA |
| MOTA | 228 | OG | SER | 29 | 37.411 | 46.697 | 49.984 | 1.00 28.74 | AAAA |
| ATOM | 229 | С | SER | 29 | 37.579 | 47.381 | 52.756 | 1.00 21.50 | AAAA |
| ATOM | 230 | Ó | SER | 29 | 38.184 | 48.320 | 53.271 | 1.00 18.95 | AAAA |
| | 231 | | LEU | 30 | | | | | |
| ATOM | | N | | | 36.256 | 47.353 | 52.673 | 1.00 19.56 | AAAA |
| MOTA | 232 | CA | LEU | 30 | 35.499 | 48.481 | 53.177 | 1.00 25.97 | AAAA |
| ATOM | 233 | CB | LEU | 30 | 34.032 | 48.396 | 52.744 | 1.00 22.90 | AAAA |
| ATOM | 234 | ÇG | LEU | 30 | 33.085 | 49.541 | 53.157 | 1.00 26.62 | AAAA |
| ATOM | 235 | | LEU | 30 | 32.885 | 49.539 | 54.648 | 1.00 38.27 | AAAA |
| | 236 | | LEU | 30 | 33.653 | | 52.698 | | |
| ATOM | | | | | | 50.885 | | 1.00 25.71 | AAAA |
| MOTA | 237 | C | LEU | 30 | 35.604 | 48.509 | 54.696 | 1.00 18.44 | AAAA |
| ATOM . | 238 | 0 | LEU | 30 | 35.704 | 49.580 | 55.273 | 1.00 25.05 | AAAA |
| ATOM | 239 | N | LEU | 31 | 35.578 | 47.336 | 55.336 | 1.00 19.65 | AAAA |
| MOTA | 240 | CA | LEU | 31 | 35.672 | 47.270 | 56.797 | 1.00 20.47 | AAAA |
| ATOM | 241 | CB | LEU | 31 | 35.613 | 45.821 | 57.300 | 1.00 20.60 | AAAA |
| | | | | | | | | | |
| ATOM | 242 | CG | LEU | 31 | 34.988 | 45.456 | 58.665 | 1.00 39.80 | AAAA |
| ATOM | 243 | | LEU | 31 | 35.712 | 44.219 | 59.257 | 1.00 23.99 | AAAA |
| MOTA | 244 | CD2 | LEU | 31 | 35.085 | 46.591 | 59.637 | 1.00 28.48 | AAAA |
| ATOM | 245 | C | LEU | 31 | 37.009 | 47.870 | 57.229 | 1.00 23.85 | AAAA |
| ATOM | 246 | 0 | LEU | 31 | 37.070 | 48.673 | 58.154 | 1.00 21.24 | AAAA |
| | | | | | | | | | |
| ATOM | 247 | N | LEU | 32 | 38.079 | 47.462 | 56.562 | 1.00 23.91 | AAAA |
| ATCM | 248 | CA | LEU | 32 | 39.400 | 47.965 | 56.899 | 1.00 24.82 | AAAA |
| ATOM | 249 | CB | LEU | 32 | 40.479 | 47.320 | 56.018 | 1.00 24.81 | AAAA |
| ATOM | 250 | CG | LEU | 32 | 40.849 | 45.854 | 56.276 | 1.00 27.00 | AAAA |
| | 251 | | LEU | 32 | 41.995 | | 55.354 | 1.00 27.13 | |
| ATOM | | | | | | 45.435 | | | AAAA |
| ATOM | 252 | | LEU | 32 | 41.285 | 45.687 | 57.720 | 1.00 34.49 | AAAA |
| MOTA | 253 | C | LEU | 32 | 39.466 | 49.475 | 56.763 | 1.00 19.56 | AAAA |
| ATOM | 254 | 0 | LEU | 32 | 39.958 | 50.143 | 57.662 | 1.00 20.71 | AAAA |
| ATOM | 255 | N | ARG | 33 | 38.974 | 50.006 | 55.645 | 1.00 23.25 | AAAA |
| | 256 | CA | | 33 | | | | 1.00 24.33 | |
| ATOM | | | ARG | | 39.007 | 51.449 | 55.441 | | AAAA |
| ATOM | 257 | CB | ARG | 33 | 38.575 | 51.806 | 54.013 | 1.00 23.46 | AAAA |
| MOTA | 258 | CG | ARG | 33 | 39.571 | 51.327 | 52.945 | 1.00 26.94 | AAAA |
| ATOM | 259 | CD | ARG | 3 3 | 39.337 | 51.976 | 51.585 | 1.00 42.13 | AAAA |
| ATOM | 260 | NE | ARG | 33 | 38.023 | 51.661 | 51.037 | 1.00 59.06 | AAAA |
| | | | | | | | | | |
| ATOM | 261 | CZ | ARG | 33 | 37.583 | 52.088 | 49.857 | 1.00 60.87 | AAAA |
| MOTA | 262 | NH1 | | 33 | 38.353 | 52.850 | 49.095 | 1.00 65.33 | AAAA |
| ATOM | 263 | NH2 | ARG | 33 | 36.373 | 51.743 | 49.433 | 1.00 56.24 | AAAA |
| ATOM | 264 | С | ARG | 33 | 38.124 | 52.156 | 56.455 | 1.00 30.33 | AAAA |
| | | | | | | | - | | , |

| _ | | | | | | | | |
|------|-------|----------|-------|--------|--------|-----------------|------------|------|
| ATOM | 265 | O ARG | 33 | 38.441 | 53.252 | 56.905 | 1.00 25.45 | AAAA |
| | | | | | | | | |
| MOTA | 266 | N PHE | 34 | 37.022 | 51.514 | 56.828 | 1.00 24.98 | AAAA |
| MOTA | 267 | CA PHE | 34 | 36.099 | 52.085 | 57.789 | 1.00 27.09 | AAAA |
| | | | | | | | | |
| ATOM | 268 | CB PHE | 34 | 34.798 | 51.276 | 57.807 | 1.00 24.88 | AAAA |
| MOTA | 269 | CG PHE | 34 | 33.719 | 51.898 | 58.631 | 1.00 20.46 | AAAA |
| | | CD1 PHE | | | | | 1.00 18.74 | |
| MOTA | | | 34 | 33.043 | 53.018 | 58.171 | | AAAA |
| MOTA | 271 | CD2 PHE | 34 | 33.396 | 51.383 | 59.889 | 1.00 20.19 | AAAA |
| | | | | | | 58.956 | | |
| MOTA | 272 | CE1 PHE | 34 | 32.043 | 53.627 | 28.920 | 1.00 23.04 | AAAA |
| MOTA | 273 | CE2 PHE | · 34. | 32.406 | 51.974 | 60.681 | 1.00 25.08 | AAAA |
| | | | | | | | | |
| MOTA | 274 | CZ PHE | 34 | 31.726 | 53.104 | 60.209 | 1.00 23.31 | AAAA |
| ATOM | 275 | C PHE | 34 | 36.709 | 52.115 | 59.194 | 1.00 23.93 | AAAA |
| | | | 34 | 36.668 | | | 1:00 21.71 | |
| ATOM | | O PHE | | | | 59.883 | | AAAA |
| ATOM | 277 | N LYS | 35 | 37.298 | 51.013 | 59.645 | 1.00 21.33 | AAAA |
| | | CA LYS | 35 | 37.862 | 51.084 | 60.978 | 1.00 22.54 | AAAA |
| MOTA | | | | | | | | |
| MOTA | 279 | CB LYS | 35 | 38.276 | 49.716 | 61.476 | 1.00 29.70 | AAAA |
| ATOM | 280 | CG LYS | 35 | 37.082 | 48.890 | 61.924 | 1.00 29.48 | AAAA |
| | | | | | | | | |
| MOTA | 281 | CD LYS | 35 | 37.517 | 47.535 | 62.398 | 1.00 42.17 | AAAA |
| ATOM | 282 | CE LYS | 35 | 38.157 | 46.762 | 61.275 | 1.00 34.89 | AAAA |
| | | | | | | | | |
| ATOM | 283 | NZ LYS | 35 | 39.372 | 47.412 | 60.719 | 1.00 67.18 | AAAA |
| ATOM | 284 | C LYS | 35 | 39.027 | 52.055 | 61.040 | 1.00 24.68 | AAAA |
| | | | | | | 62.085 | | |
| MOTA | 285 | O LYS | 35 | 39.282 | 52.640 | | 1.00 22.33 | AAAA |
| MOTA | 286 | N ASP | 36 | 39.724 | 52.231 | 59.926 | 1.00 25.67 | AAAA |
| | | | 36 | 40.842 | 53.163 | 59.898 | 1.00 25.57 | |
| MOTA | | | | | • | | | AAAA |
| MOTA | 288 | CB ASP | 36 | 41.669 | 52.984 | 58.621 | 1.00 32.26 | AAAA |
| ATOM | 289 | CG ASP | 36 | 42.881 | 53.914 | 58.572 | 1.00 33.92 | AAAA |
| | _ | | | | | | | |
| MOTA | 290 | OD1 ASP | 36 | 43.641 | 53.969 | 59.563 | 1.00 40.22 | AAAA |
| ATOM | 291 | OD2 ASP | 36 | 43.078 | 54.575 | 57.538 | 1.00 40.06 | AAAA |
| | | | | | | | | |
| MOTA | 292 (| C ASP | 36 | 40.285 | 54.578 | 59.973 | 1.00 28.04 | AAAA |
| MOTA | 293 (| O ASP | 36 | 40.761 | 55.397 | 60.765 | 1.00 29.52 | AAAA |
| | | ALA V | 37 | 39.272 | 54.864 | 59.159 | 1.00 23.32 | AAAA |
| ATOM | | | | | | | | |
| MOTA | 295 (| CA ALA | 37 | 38.651 | 56.192 | 59.163 | 1.00 28.22 | AAAA |
| ATOM | 296 | CB ALA | 37 | 37.506 | 56.251 | 58.119 | 1.00 25.93 | AAAA |
| | | | | | | | | |
| ATOM | 297 (| C ALA | 37 | 38.127 | 56.549 | 60.565 | 1.00 28.41 | AAAA |
| ATOM | 298 (| O ALA | 37 | 38.186 | 57.708 | 60.972 | 1.00 29.27 | AAAA |
| | | MET. | 38 | 37.639 | 55.547 | 61.300 | 1.00 24.76 | AAAA |
| ATOM | | | | | | | | |
| ATOM | 300 (| CA MET | 38 | 37.103 | 55.727 | 62.669 | 1.00 25.45 | AAAA |
| ATOM | 301 (| CB MET | 38 | 36.077 | 54.625 | 62.982 | 1.00 25.19 | AAAA |
| | | | | | | | | |
| MOTA | 302 (| G MET | 38 | 34.816 | 54.660 | 62.148 | 1.00 22.32 | AAAA |
| ATOM | 303 9 | D MET | 38 | 33.733 | 55.983 | 62.702 | 1.00 29.90 | AAAA |
| | | | | | | 64.376 | 1.00 26.51 | |
| MOTA | | CE MET | 38 | 33.402 | 55.417 | | | AAAA |
| ATOM | 305 (| MET | 38 | 38.203 | 55.667 | 63.744 | 1.00 26.42 | AAAA |
| ATOM | 306 |) MET | 38 | 37.924 | 55.818 | 64.947 | 1.00 23.77 | AAAA |
| | | | | | | | | |
| ATOM | 307 N | i asn | 39 | 39.437 | 55.434 | 63.300 | 1.00 26.21 | AAAA |
| ATOM | 308 (| A ASN | 39 | 40.607 | 55.308 | 64.170 | 1.00 28.53 | AAAA |
| | | B ASN | 39 | 40.926 | 56.643 | 64.855 | 1.00 33.95 | AAAA |
| MOTA | | | | | | | | |
| ATOM | 310 C | G ASN | 39 | 41.153 | 57.751 | 63 .8 58 | 1.00 29.46 | AAAA |
| | 311 0 | D1 ASN | 39 | 41.930 | 57.596 | 62.925 | 1.00 36.28 | AAAA |
| MOTA | | | | | | | | |
| ATOM | 312 N | ID2 ASN | 39 | 40.472 | 58.880 | 64.046 | 1.00 40.03 | AAAA |
| ATOM | 313 C | ASN | 39 | 40.374 | 54.223 | 65.205 | 1.00 30.07 | AAAA |
| | 314 C | | 39 | 40.682 | 54.390 | 66.395 | 1.00 25.47 | AAAA |
| ATOM | | | | | | | | |
| ATOM | 315 N | LEU | 40 | 39.814 | 53.105 | 54.744 | 1.00 28.19 | AAAA |
| | 316 C | A LEU | 40 | 39.527 | 51.984 | 65.633 | 1.00 25.50 | AAAA |
| ATOM | | | | | | | | |
| ATOM | 317 C | B LEU | 40 | 38.060 | 51.562 | 65.514 | 1.00 32.14 | AAAA |
| MOTA | 318 C | G LEU | 40 | 37.044 | 52.585 | 66.036 | 1.00 30.47 | AAAA |
| | | | | | | | 1.00 29.07 | AAAA |
| MOTA | | D1 LEU | 40 | 35.637 | 52.027 | 65.894 | | |
| MOTA | 320 C | D2 LEU | 40 | 37.325 | 52.889 | 67.491 | 1.00 23.80 | AAAA |
| | 321 C | | 40 | 40.433 | 50.771 | 65.415 | 1.00 26.99 | AAAA |
| ATOM | | | | | | | | |
| MOTA | 322 0 | LEU | 40 | 40.157 | 49.683 | 65.915 | 1.00 25.41 | AAAA |
| ATOM | 323 N | | 41 | 41.528 | 50.970 | 64.691 | 1.00 28.33 | AAAA |
| | | | | | | | | |
| ATOM | 324 C | A ILE | 41 | 42.459 | 49.882 | 64.459 | 1.00 25.08 | AAJA |
| ATCM | 325 C | B ILE | 41 | 42.010 | 49.020 | 63.243 | 1.00 25.01 | AAAA |
| | | | | | | 61.961 | 1.00 22.74 | AAAA |
| MOTA | | G2 ILE | 41 | 42.061 | 49.824 | | | |
| ATOM | 327 C | G1 ILE | 41 | 42.917 | 47.802 | 63.128 | 1.00 31.01 | AAAA |
| - | | D1 ILE | 41 | 42.895 | 46.951 | 64.341 | 1.00 42.18 | AAAA |
| ATCM | | | | | | | | |
| ATOM | 329 C | ILE | 41 | 43.900 | 50.376 | 64.247 | 1.00 24.09 | AAAA |
| • | 330 0 | ILE | 41 | 44.128 | 51.406 | 63.621 | 1.00 28.92 | AAAA |
| ATOM | | معابيد ي | | | 32.300 | | | |
| | | - | | | • | | | - |

| MOTA | 331 N ASP | 42 | 44.86 | 6 49.63 | 4 64.787 | 1.00 28.95 | AAAA |
|--------------|--------------------------|----------|------------------|------------------|------------------|------------|--------------|
| MOTA | 332 CA ASP | 42 | 46.27 | | | | AAAA |
| MOTA | 333 CB ASP | 42 | 46.95 | L 50.09 | | | AAAA |
| ATOM | 334 CG ASP | 42 | 46.26 | | | | AAAA |
| ATOM | 335 OD1 ASP | 42 | 46.079 | | | | |
| ATOM | 336 OD2 ASP | 42 | 45.924 | | | | AAAA |
| ATOM | 337 C ASP | 42 | 46.985 | | | | AAAA |
| ATOM | 338 O ASP | 42 | 46.594 | | | | AAAA . |
| ATOM | 339 N GLU | 43 | 48.036 | | | | AAAA |
| ATOM | 340 CA GLU | 43 | 48.793 | | | | AAAA |
| ATOM | 341 CB GLU | 43 | 50.078 | | | | AAAA |
| MOTA | 342 CG GLU | 43 | 49.886 | | | | AAAA |
| MOTA | 343 CD GLU | 43 | 51.214 | | | 1.00 60.39 | AAAA |
| ATOM | 344 OE1 GLU | 43 | 51.928 | | _ | 1.00 70.32 | AAAA |
| ATOM | 345 OE2 GLU | 43 | 51.550 | | | 1.00 60.38 | AAAA |
| ATOM | 346 C GLU | 43 | 49.196 | | | 1.00 38.04 | AAAA |
| ATOM | 347 O GLU | 43 | 49.125 | | | 1.00 36.83 | AAAA |
| ATOM | 348 N LYS | 44 | 49.636 | | | 1.00 28.26 | AAAA |
| MOTA | 349 CA LYS | 44 | 50.084 | | | 1.00 32.71 | AAAA |
| MOTA | 350 CB LYS | 44 | 50.974 | | | 1.00 44.28 | AAAA |
| MOTA | 351 CG LYS | 44 | 52.211 | 47.007 | | 1.00 59.37 | AAAA |
| MOTA | 352 CD LYS | 44 | 53.187 | 47.449 | | 1.00 68.87 | AAAA |
| MOTA | 353 CE LYS | 44 | 54.373 | 48.167 | | 1.00 67.21 | AAAA |
| ATOM | 354 NZ LYS | 44 | 55.361 | 48.648 | | 1.00 74.00 | AAAA |
| ATOM | 355 C LYS | 44 | 48.982 | 44.889 | | 1.00 26.75 | AAAA AAAA |
| ATOM | 356 O LYS | 44 | 49.265 | 43.792 | | 1.00 27.37 | AAAA |
| MOTA | 357 N GLU | 45 | 47.731 | 45.278 | | 1.00 29.20 | AAAA |
| ATOM | 358 CA GLU | 45 | 46.580 | 44.414 | 65.165 | 1.00 21.58 | AAAA |
| ATOM | 359 CB GLU | 45 | 45.387 | 45.243 | 65.676 | 1.00 18.24 | AAAA |
| MOTA | 360 CG GLU | 45 | 45.551 | 45.828 | 67.077 | 1.00 26.57 | AAAA |
| MOTA | 361 CD GLU | 45 | 44.418 | 46.772 | 67.453 | 1.00 23.12 | AAAA |
| MOTA | 362 OE1 GLU | 45 | 44.224 | 47.783 | 66.746 | 1.00 21.64 | AAAA |
| MOTA | 363 OE2 GLU | 45 | 43.725 | 46.509 | 68.454 | 1.00 26.48 | AAAA |
| ATOM | 364 C GLU | 45 . | 46.163 | 43.710 | 63.870 | 1.00 26.31 | AAAA |
| ATOM | 365 O GLU | 45 | 45.400 | 42.739 | 63.889 | 1.00 22.32 | AAAA |
| MOTA | 366 N LEU | 46 | 46.674 | 44.204 | 62.748 | 1.00 20.15 | AAAA |
| ATOM | 367 CA LEU | 46 | 46.317 | 43.642 | 61.448 | 1.00 25.80 | AAAA |
| ATOM | 368 CB LEU | 46 | 46.137 | 44.774 | 60.433 | 1.00 27.25 | AAAA |
| ATOM | 369 CG LEU | 46 | 45.763 | 44.397 | 58.997 | 1.00 37.72 | AAAA |
| ATOM | 370 CD1 LEU | 46 | 44.356 | 43.810 | 58.984 | 1.00 39.46 | AAAA |
| ATOM | 371 CD2 LEU 372 C LEU | 46 | 45.822 | 45.632 | 58.101 | 1.00 35.43 | AAAA |
| ATOM ATOM | _ | 46 | 47.305 | 42.623 | 60.896 | 1.00 28.88 | AAAA |
| ATOM | 373 O LEU 374 N ILE | 46 | 48.513 | 42.860 | 60.862 | 1.00 31.98 | AAAA |
| ATOM | | 47 | 46.791 | 41.469 | 60.482 | 1.00 16.92 | AAAA |
| ATOM | 375 CA ILE 376 CB ILE | 47 47 | 47.638 | 40.448 | 59.872 | 1.00 20.98 | · AAAA |
| ATOM | 377 CG2 ILE | 47 | 47.412 | 39.046 | 67.513 | 1.00 21.51 | AAAA |
| ATOM | 378 CG1 ILE | 47 | 48.115 47.947 | 37.958 39.040 | 52.696 | 1.00 20.32 | AAAA |
| ATOM | 379 CD1 FLE | 47 | 49.450 | 39.207 | 6 .950 | 1.00 20.71 | AAAA |
| ATOM | 380 C ILE | 47 | 47.227 | | 62.052 | 1.00 38.87 | AAAA |
| ATOM | 381 O ILE | 47 | 46.036 | 40.417 | 58.406 58.101 | 1.00 24.50 | AAAA |
| ATOM | 382 N LYS | 48 | 48.195 | 40.279 40.550 | | 1.00 20.74 | AAAA |
| ATOM | 383 CA LYS | 48 | 47.883 | 40.543 | 57.500 | 1.00 18.73 | AAAA |
| ATOM | 384 CB LYS | 48 | 49.095 | 40.991 | 56.072 55.239 | 1.00 15.55 | AAAA |
| ATOM | 385 CG LYS | 48 | 48.836 | 41.011 | | 1.00 16.52 | AAAA |
| ATOM | 386 CD LYS | 48 | 50.072 | 41.451 | 53.738 52.957 | 1.00 23.25 | AAAA |
| ATOM | 387 CE LYS | 18 | 49.796 | 41.496 | | 1.00 32.69 | AAAA |
| ATOM | 388 NZ LYS | 48 | 48.704 | 42.449 | 51.462 | 1.00 26.00 | AAAA |
| ATOM | 389 C LYS | 18 | 47.473 | 39.140 | 51.114 | 1.00 46.33 | AAAA |
| ATOM | 390 O LYS | 48 | 48.177 | 38.174 | 55.629 | 1.00 14.43 | AAAA |
| ATCM | 391 N SER | 19 | 46.343 | 39.049 | 55.887 | 1.00 16.83 | AAAA |
| ATOM | 392 CA SER | 49 | 45.838 | 37.780 | 54.945 | 1.00 16.61 | AAAA |
| ATOM | 393 CB SER | 49 | 44.517 | 37.780 | 54.439 | 1.00 14.33 | AAAA |
| ATOM | 394 OG SER | 49 | 43.509 | | 53.694 | 1.00 13.21 | AAAA |
| ATOM | 395 C SER | 49 | 46.810 | 38.613 37.131 | 54.492 | 1.00 16.86 | AAAA |
| ATOM | 396 O SER | 49 | 47.463 | 37.131 | 53.459 | 1.00 24.11 | AAAA |
| | · · | | 31.505 | J1.013 | 52.663 | 1.00 19.59 | AAAA |
| | | | | | | | |

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Figure 16-7

| • | | | | | | | | • | |
|--------|------------|-----|-------|-----------------|--------|---------------------|------------------|------------|------|
| MOTA | 397 | N | ARG | 50 | 46.890 | 35.805 | 53.519 | 1.00 16.83 | AAAA |
| ATOM | 398 | CA | ARG | 50 | 47.724 | 35.037 | 52.610 | 1.00 23.88 | AAAA |
| | 399 | | · ARG | 50 | 48.805 | 34.247 | 53.366 | 1.00 27.48 | AAAA |
| MOTA | 400 | CG | ARG | 50 | 48.284 | 33.036 | 54.177 | 1.00 22.99 | AAAA |
| ATOM | 401 | CD | ARG | 50 | 49.453 | 32.263 | 54.759 | 1.00 25.20 | AAAA |
| ATOM | | | | | 49.073 | 31.197 | 55.684 | 1.00 15.88 | AAAA |
| ATOM | 402 | NE | ARG | 50 | | 30.093 | 55.368 | 1.00 14.34 | AAAA |
| MOTA | 403 | CZ | ARG | 50 | 48.411 | | 54.117 | 1.00 15.78 | AAAA |
| MOTA | 404 | | ARG | 50 ' | 48.023 | 29.863 | | | AAAA |
| ATOM | 405 | | ARG | 50 | 48.150 | 29.197 | 56.312 | 1.00 16.78 | |
| MOTA | 406 | С | ARG | 50 | 46.821 | 34.023 | 51.905 | 1.00 20.20 | AAAA |
| MOTA | 407 | 0 | ARG | 50 - | 45.763 | 33.650 | 52.414 | 1.00 18.63 | AAAA |
| ATOM . | 408 | N | PRO | 51 | 47.203 | 33.596 | 50.699 | 1.00 15.63 | AAAA |
| ATOM | 409 | CD | PRO | 51 | 48.322 | 34.028 | 49.850 | 1.00 19.45 | AAAA |
| ATOM | 410 | CA | PRO | 51 | 46.387 | ··32:606 | 49.994 | 1.00 14.35 | AAAA |
| ATOM | 411 | CB | PRO | 51 · | 47.076 | 32.514 | 48.629 | 1.00 17.73 | AAAA |
| ATOM | 412 | CG | PRO | 51 | 47.707 | . 33.890 | 48.475 | 1.00 17.62 | AAAA |
| ATOM | 413 | C | PRO | 51 | 46.452 | 31.256 | 50.708 | 1.00 15.73 | AAAA |
| ATOM | 414 | 0 | PRO | 51 | 47.460 | 30.942 | 51.350 | 1.00 18.67 | AAAA |
| ATOM | 415 | N | ALA | 52 | 45.377 | 30.470 | 50.618 | 1.00 11.47 | AAAA |
| MOTA | 416 | CA | ALA | 52 | 45.375 | 29.117 | 51.161 | 1.00 9.78 | AAAA |
| | 417 | CB | ALA | 52 | 43.967 | 28.529 | 51.112 | 1.00 12.19 | AAAA |
| MOTA | 418 | c | ALA | 52 | 46.301 | 28.342 | 50.209 | 1.00 17.19 | AAAA |
| MOTA | 419 | Ö | ALA | 52 | 46.307 | | 49.006 | 1.00 16.46 | AAAA |
| ATOM | | Ŋ | THR | 53 | 47.081 | 27.392 | 50.723 | 1.00 16.40 | AAAA |
| MOTA | 420 | CA | THR | 53 | 47.952 | 26.615 | 49.843 | 1.00 16.32 | AAAA |
| MOTA | 421 422 | CB | THR | 53 _. | 49.109 | 25.959 | 50.612 | 1.00 15.82 | AAAA |
| MOTA | | | THR | 53 53 | 48.582 | 25.016 | 51.559 | 1.00 16.25 | AAAA |
| MOTA | 423 | | | | 49.923 | 27.030 | 51.336 | 1.00 14.34 | AAAA |
| ATOM | 424 | CG2 | | 53 53 | 47.104 | 25.520 | 49.215 | 1.00 14.06 | AAAA |
| MOTA | 425 | C | THR | | 46.012 | 25.241 | 49.690 | 1.00 17.87 | AAAA |
| MOTA | 426 | 0 | THR | 53 | 47.599 | 24.903 | 48.145 | 1.00 16.10 | AAAA |
| MOTA | 427 | N | LYS. | | 46.848 | 23.832 | 47.492 | 1.00 19.00 | AAAA |
| MOTA | 428 | CA | LYS | 54 | | 23.245 | | 1.00 22.92 | AAAA |
| ATOM | 429 | CB | LYS | 54 | 47.671 | | 45.539 | 1.00 22.32 | AAAA |
| ATOM | 430 | .CG | LYS | 54 | 46.955 | 22.172 | | 1.00 51.34 | AAAA |
| ATOM | 431 | CD | LYS | 54 | 45.787 | 22.733 | 44.757 43.561 | 1.00 51.54 | AAAA |
| MOTA | 432 | CE | LYS | 54 | 46.244 | 23.565 | | 1.00 63.45 | AAAA |
| ATOM | 433 | NZ | LYS | 54 | 46.898 | 22.733 | 42.505 | 1.00 03.43 | AAAA |
| MOTA | 434 | C | LYS | 54 | 46.554 | 22.738 | 48.520 | 1.00 22.48 | AAAA |
| MOTA | 435 | 0 | LYS | 54 | 45.463 | 22.158 | 48.555 | 1.00 15.57 | AAAA |
| ATOM | 436 | N | GLU | 55 | 47.536 | 22.465 | 49.364 | | AAAA |
| MOTA | 437 | CA | GLU | 55 | 47.389 | 21.432 | 50.383 | 1.00 25.08 | AAAA |
| MOTA | 438 | CB | GLU | 55 | 48.718 | 21.241 | 51.116 | 1.00 25.40 | AAAA |
| ATOM | 439 | CG | GLU | 55 | 48.703 | 20.185 | 52.199 | 1.00 48.95 | |
| ATOM | 440 | CD | GLU | 55 | 50.106 | 19.821 | 52.673 | 1.00 64.21 | AAAA |
| ATOM | 441 | OE1 | GLU | 55 | 50.220 | 19.033 | 53.640 | 1.00 62.38 | AAAA |
| ATOM | 42 | OE2 | GLU | 55 | 51.093 | 20.311 | 52.073 | 1.00 58.22 | AAAA |
| ATOM | .43 | С | GLU | 55 | 46.273 | 21.773 | 51.362 | 1.00 18.91 | AAAA |
| ATOM | -44 | 0 | GLU | 55 | 45.489 | 20.908 | 51.723 | 1.00 17.43 | AAAA |
| ATOM | 445 | N | GLU | 56 | 46.196 | 23.029 | 51.786 | 1.00 16.80 | AAAA |
| ATOM | 446 | CA | GLU | 56 | 45.137 | 23.432 | 52.698 | 1.00 17.24 | AAAA |
| ATOM | 447 | CB | GLU | 56 | 45.399 | 24.855 | 53.204 | 1.00 16.15 | AAAA |
| MOTA | 448 | CG | GLU | 56 | 46.709 | 24.941 | 54.009 | 1.00 14.41 | AAAA |
| MOTA | 449 | CD | GLU | 56 | 47.087 | 26.354 | 54.358 | 1.00 20.17 | AAAA |
| MOTA | 450 | OE1 | GLU | 56 · | 46.713 | 27.252 [.] | 53.567 | 1.00 17.12 | AAAA |
| MOTA | 451 | | GLU | 56 | 47.773 | 26.564 | 55.394 | 1.00 18.23 | AAAA |
| MOTA | 452 | C | GLU | 56 | 43.781 | 23.313 | 52.000 | 1.00 15.95 | AAAA |
| | 453 | ō | GLU | 56 | 42.799 | 22.869 | 52.599 | 1.00 17.82 | AAAA |
| MOTA | 454 | N | LEU | 57 | 43.722 | 23.691 | 50.725 | 1.00 17.53 | AAAA |
| MOTA | 455 | CA | LEU | 5 <i>7</i> | 42.466 | 23.579 | 49.989 | 1.00 16.34 | AAAA |
| MOTA | 456 | CB | LEU | 57 | 42.591 | 24.177 | 48.586 | 1.00 13.86 | AAAA |
| MOTA | | CG | LEU | 57 | 42.773 | 25.707 | 48.552 | 1.00 15.24 | AAAA |
| ATOM | 457 | | LEU | 57 57 | 42.923 | 26.182 | 47,101 | 1.00 19.30 | AAAA |
| ATOM | 458 | | | 57 57 | 41.546 | 26.380 | 49.207 | 1.00 15.14 | AAAA |
| ATOM | 459 | | LEU | | 42.016 | 22.126 | 49.868 | 1.00 18.46 | AAAA |
| MOTA | 460 | C | LEU | 57 57 | 40.824 | 21.823 | | 1.00 17.27 | AAAA |
| ATOM | 461 | 0 | LEU | 57 58 | | 21.234 | 49.636 | 1.00 16.43 | AAAA |
| ATOM | 462 | N . | LEU | 58 | 42.975 | Z1.Z24 | - | 2 20 | |
| | | | | | | | | | |

SUBSTITUTE SHEET (RULE 26)

Figure 16-8

| MOTA | 463 CA LEU | J 58 | 42.66 | 2 19.822 | 49:475 | 1.00 15.18 | AAAA |
|--------------|--------------------------|----------|------------------|------------------|------------------|--------------------------|--------------|
| MOTA | 464 CB LEU | J 58 | 43.78 | | | | AAAA |
| MOTA | 465 CG LEU | 58 | 44.02 | 9 19.682 | | | AAAA |
| MOTA | 466 CD1 LEU | .58 | 45.22 | 18.982 | | | AAAA |
| ATOM | 467 CD2 LEU | 58 | 42.786 | 5 19.549 | | | AAAA |
| ATOM | 468 C LEU | 58 | 42.339 | 9 19.116 | | | AAAA |
| ATOM | 469 O LEU | 58 | 42.067 | 7 17.914 | | | AAAA |
| ATOM | 470 N LEU | 59 | 42.377 | 7 19.849 | 51.896 | | AAAA |
| MOTA | 471 CA LEU | 59 | 41.958 | 3 19.261 | | | AAAA |
| MOTA | 472 CB LEU | 59 | 42.182 | | | | AAAA |
| ATOM | 473 CG LEU | 59 | 43.619 | 20.537 | | 1.00 22.57 | AAAA |
| MOTA | 474 CD1 LEU | | 43.640 | 21.654 | 55.808 | 1.00 19.88 | AAAA |
| MOTA | 475 CD2 LEU | | 44.255 | 19.253 | | 1.00 26.71 | AAAA |
| ATOM | 476 C LEU | | 40.446 | | 53.043 | 1.00 17.55 | AAAA |
| MOTA | 477 O LEU | | 39.897 | 18.112 | 53.724 | 1.00 18.02 | AAAA |
| MOTA | 478 N PHE | 60 . | 39.766 | 19.737 | 52.179 | 1.00 14.64 | - AAAA |
| ATOM | 479 CA PHE | 60 | 38.338 | 19.536 | 51.970 | 1.00 18.17 | AAAA |
| ATOM | 480 CB PHE | 60 | 37.519 | 20.694 | | 1.00 18.80 | AAAA |
| MOTA | 481 CG PHE | 60 | 36.028 | | 52.316 | 1.00 15.94 | AAAA |
| ATOM | 482 CD1 PHE | 60 | 35.320 | | 52.817 | 1.00 19.98 | AAAA |
| ATOM | 483 CD2 PHE | 60 | 35.339 | | 51.576 | 1.00 18.09 | AAAA |
| ATOM | 484 CE1 PHE | 60 | 33.947 | | 52.587 | 1.00 18.72 | AAAA |
| ATOM | 485 CE2 PHE | 60 | 33.964 | 21.399 | 51.338 | 1.00 19.19 | AAAA |
| ATOM | 486 CZ PHE | 60 | 33.268 | 20.295 | 51.850 | 1.00 18.43 | AAAA |
| ATOM | 487 C PHE 488 O PHE | 60 | 37.916 | 19.337 | 50.510 | 1.00 16.45 | AAAA |
| MOTA MOTA | 489 N HIS | 60 . | 37.227 | 18.371 | 50.179 | 1.00 19.18 | AAAA |
| ATOM | 490 CA HIS | 61 61 | 38.308 | 207.257 | | 1.00 18.26 | AAAA |
| MOTA | 491 CB HIS | 61 | 37.913 38.004 | 20.163 | 48.235 | 1.00 14.47 | AAAA |
| ATOM | 492 CG HIS | 61 | 36.968 | 21.545 22.494 | 47.582 | 1.00 17.15 | AAAA |
| ATOM | 493 CD2 HIS | 61 | 35.645 | 22.580 | 48.084 47.816 | 1.00 14.20 1.00 11.05 | AAAA |
| ATOM | 494 ND1 HIS | 61 | 37.237 | 23.477 | 49.012 | 1.00 11.05 | AAAA |
| ATOM | 495 CE1 HIS | 61 | 36.121 | 24.131 | 49.291 | 1.00 23.25 | AAAA |
| ATOM | 496 NE2 HIS | 61 | 35.143 | 23.606 | 48.579 | 1.00 21.07 | AAAA AAAA |
| MOTA | 497 C HIS | 61 | 38.695 | 19.157 | 47.417 | 1.00 18.29 | AAAA |
| ATOM | 498 O HIS | 61 | 39.828 | 18.819 | 47.761 | 1.00 17.50 | AAAA |
| ATOM | 499 N THR | 62 | 38.071 | 18.658 | 46.346 | 1.00 15.39 | AAAA |
| ATOM | 500 CA THR | 62 | 38.741 | 17.686 | 45.473 | 1.00 19.02 | AAAA |
| ATOM | 501 CB THR | 62 | 37.734 | 16.767 | 44.756 | 1.00 19.61 | AAAA |
| ATOM | 502 OG1 THR | 62 | 36.795 | 17.548 | 44.006 | 1.00 22.05 | AAAA |
| ATOM | 503 CG2 THR | 62 | 36.995 | 15.925 | 45.767 | 1.00 28.99 | AAAA |
| MOTA | 504 C THR | 62 | 39.595 | 18.398 | 44.440 | 1.00 23.22 | AAAA |
| ATOM | 505 O THR | 62 | 39.311 | 19.532 | 44.044 | 1.00 17.47 | AAAA |
| ATOM | 506 N GLU | 63 | 40.657 | 17.732 | 44.009 | 1.00 18.94 | AAAA |
| MOTA | 507 CA GLU 508 CB GLU | 63 | 41.571 | 18.324 | 43.046 | 1.00 22.44 | AAAA |
| ATOM | 509 CG GLU | 63 | 42.736 | 17.384 | 42.750 | 1.00 28.31 | AAAA |
| MOTA MOTA | 510 CD GLU | 63 63 | 43.885 | 17.476 | 43.708 | 1.00 60.37 | AAAA |
| ATOM | 511 OE1 GLU | 63 | 45.154 45.603 | 16.893 | 43.115 | 1.00 65.08 | AAAA |
| ATOM | 512 OE2 GLU | 63 | 45.697 | 17.407 | 42.065 | 1.00 66.44 | AAAA |
| ATOM | 513 C GLU | 63 | 40.983 | 15.927 18.764 | 43.694 | 1.00 71.72 | AAAA |
| ATOM | 514 O GLU | 63 | 41.340 | 19.827 | 41.730 41.228 | 1.00 18.63 | AAAA |
| ATOM | 515 N ASP | 64 | 40.108 | 17.943 | 41.228 | 1.00 18.37 1.00 19.77 | AAAA |
| ATOM | 515 CA ASP | 64 | 39.508 | 18.277 | 39.864 | 1.00 17.88 | AAAA |
| MOTA | 517 CB ASP | 64 | 38.584 | 17.159 | 39.372 | 1.00 17.88 | AAAA |
| ATOM | 518 .CG ASP | 64 | 37.429 | 16.884 | 40.330 | 1.00 20.43 | AAAA AAAA |
| ATOM | 519 OD1 ASP | 64 | 36.415 | 16.291 | 39.899 | 1.00 45.01 | AAAA |
| ATOM | 520 OD2 ASP | 64 | 37.537 | 17.243 | 41.521 | 1.00 43.01 | AAAA |
| ATOM | 521 C ASP | 64 | 38.701 | 19.582 | 39.964 | 1.00 31.77 | AAAA |
| ATOM | 522 O ASP | 64 . | 38.726 | 20.410 | 39.042 | 1.00 21.30 | AAAA |
| ATOM | 523 N TYR | 65 | 37.980 | 19.750 | 41.072 | 1.00 16.17 | AAAA |
| ATOM | 524 CA TYR | 65 | 37.178 | 20.957 | 41.292 | 1.00 15.62 | AAAA |
| ATOM | 525 CB TYR | 65 | 36.258 | 20.796 | 42.529 | 1.00 12.04 | AAAA |
| ATOM | 526 CG TYR | 65 | 35.501 | 22.065 | 42.886 | 1.00 12.23 | AAAA |
| ATOM | 527 CD1 TYR | 65 | 34.699 | 22.718 | 41.940 | 1.00 14.73 | AAAA |
| ATOM | 528 CE1 TYR | 65 | 34.028 | 23.910 | 42.253 | 1.00 18.23 | AAAA |
| • | | | | _ | _ | | |

27/263 Figure 16-9

| | | | | | _ | | | | |
|--------|--------------|-----|------|-----------------|--------|--------|--------|------------|--------|
| MOTA | 529 | CD2 | TYR | 65 | 35.609 | 22.631 | 44.163 | 1.00 13.67 | AAAA |
| MOTA | 530 | CE2 | TYR | 65 | 34.943 | 23.824 | 44.486 | 1.00 18.16 | AAAA |
| | | | | | | 24.461 | 43.533 | 1.00 16.88 | AAAA |
| ATOM | 531 | CZ. | TYR | 65. | 34.162 | | | | • |
| MOTA | 532 | OH | TYR | 65 | 33.555 | 25.665 | 43.837 | 1.00 14.59 | AAAA |
| | 533 | С | TYR | 65 | 38.090 | 22.177 | 41.459 | 1.00 15.27 | AAAA |
| MOTA | | | | | | 23.189 | 40.798 | 1.00 15.96 | AAAA |
| ATOM | 534 | 0 | TYR | _. 65 | 37.882 | | | | |
| MOTA | 535 | N | ILE | 66 | 39.098 | 22.073 | 42.321 | 1.00 14.29 | AAAA |
| | 536 | CA | ILE | 66 | 40.022 | 23.179 | 42.540 | 1.00 18.86 | AAAA |
| MOTA | | | | | | | | 1.00 15.56 | AAAA |
| MOTA | 537 | CB | ILE | 66 | 41.090 | 22.836 | 43.617 | | |
| ATOM | 538 | CG2 | ILE | 66 | 42.152 | 23.943 | 43.698 | 1.00 20.45 | AAAA |
| | | CG1 | | 66 | 40.405 | 22.659 | 44.967 | 1.00 19.68 | AAAA |
| MOTA | 539 | | | | | | 45.454 | 1.00 29.11 | · AAAA |
| MOTA | 540 | CD1 | ILE | 66 | 39.717 | 23.948 | | | |
| MOTA | 541 | С | ILE | 66 | 40.716 | 23.519 | 41.236 | 1.00 25.20 | AAAA . |
| | 542 | O | ILE | 66 | 40.809 | 24.692 | 40.895 | 1.00 14.60 | AAAA |
| MOTA | | | | | | | 40.498 | 1.00 18.21 | AAAA |
| MOTA | 543 | N | ASN | 67 | 41.190 | 22.508 | | | |
| ATOM | 544 | CA | ASN | 67 | 41.879 | 22.789 | 39.236 | 1.00 20.03 | AAAA |
| | 545 | CB | ASN | 67 | 42.448 | 21.523 | 38.580 | 1.00 21.73 | AAAA |
| ATOM | | | | | | 20.954 | 39.333 | 1.00 21.69 | AAAA |
| ATOM | 546 | CG | ASN | 67 | 43.645 | | | · | |
| ATOM | 547 | OD1 | ASN | 67 | 44.293 | 21.645 | 40.110 | 1.00 23.97 | AAAA |
| | 548 | ND2 | 2 SN | 67 | 43.947 | 19.692 | 39.086 | 1.00 23.23 | AAAA |
| MOTA | | | | | 40.970 | 23.500 | 38.250 | 1.00 15.87 | AAAA |
| MOTA | 549 | С | ASN | 67 | | | | | |
| ATOM | 550 | 0 | ASN | 67 | 41.431 | 24.347 | 37.473 | 1.00 18.64 | AAAA |
| MOTA | 551 | N | THR | 68 | 39.681 | 23.180 | 38.295 | 1.00 16.55 | AAAA |
| | | | THR | 68 | 38.729 | 23.814 | 37.400 | 1.00 20.34 | AAAA |
| ATOM | 552 | CA | | | | | | 1.00 22.99 | AAAA |
| MOTA | 553 | CB | THR | 68 | 37.360 | 23.114 | 37.441 | | |
| ATOM | 554 | OG1 | THR | 68 | 37.511 | 21.760 | 36.978 | 1.00 21.75 | AAAA |
| | 555 | CG2 | | 68 | 36.378 | 23.827 | 36.536 | 1.00 17.37 | AAAA |
| ATOM | | | | | | | 37.755 | | AAAA |
| ATOM | 556 | С | THR | 68 . | 38.561 | 25.291 | | | |
| MOTA | 5 5 7 | 0 | THR | 68 | 38.472 | 26.139 | 36.871 | 1.00 18.79 | AAAA |
| ATOM | 558 | N | LEU | 69 | 38.534 | 25_604 | 39.045 | 1.00 14.82 | AAAA |
| | | | | 69 | 38.405 | 27.000 | 39.447 | 1.00 15.20 | AAAA |
| MOTA | 559 | CA | LEU | | | | | 1.00 16.87 | AAAA |
| ATOM | 560 | CB | LEU | 69 | 38.295 | 27.126 | 40.973 | | |
| ATOM | 561 | CG | LEU | 69 | 37.057 | 26.551 | 41.666 | 1.00 14.76 | AAAA |
| | 562 | CD1 | | 69 | 37.212 | 26.643 | 43.179 | 1.00 16.81 | AAAA |
| MOTA | | | | | | | 41.217 | 1.00 17.26 | AAAA |
| MOTA | 563 | CD2 | | 69 | 35.832 | 27.312 | | | AAAA |
| ATOM | 564 | С | LEU | 69 | 39.623 | 27.796 | 38.969 | 1.00 15.11 | |
| ATOM | 565 | 0 | LEU | 69 | 39.500 | 28.934 | 38.504 | 1.00 13.30 | AAAA |
| | | | | 70 | 40.803 | 27.204 | 39.090 | 1.00 13.40 | AAAA |
| ATOM | 566 | N | MET | | | | | 1.00 16.97 | AAAA |
| MOTA | 567 | CA | MET | 70 | 42.019 | 27.894 | 38.659 | | |
| ATOM . | 568 | CB | MET | 70 | 43.254 | 27.114 | 39.075 | 1.00 14.87 | AAAA |
| | | CG | MET | 70 | 43.335 | 26.886 | 40.582 | 1.00 15.18 | AAAA |
| MOTA | 569 | | | | | | 41.060 | 1.00 28.71 | AAAA |
| ATOM | 570 | SD | MET | 70 | 44.828 | 25.954 | | | |
| ATOM | 5 71 | CE | MET | 70 | 46.051 | 27.228 | 40.893 | 1.00 21.19 | AAAA |
| ATOM | 572 | С | MET | 70 | 42.064 | 28.119 | 37.155 | 1.00 19.11 | AAAA |
| | | | | 70 | 42.498 | 29.170 | 36.700 | 1.00 17.10 | AAAA |
| ATOM | 573 | 0 | MET | | | | | 1.00 15.06 | AAAA |
| ATOM | 574 | N | GLI | 71 | 41.648 | 27.118 | 36.389 | | |
| ATOM | 5 75 | CA | GLu | 71 | 41.651 | 27.226 | 34.934 | 1.00 16.12 | AAAA |
| | 576 | CB | GLi | 71 | 41.397 | 25.856 | 34.305 | 1.00 16.12 | AAAA |
| MOTA | | | | | | 25.882 | 32,800 | 1.00 20.26 | AAAA |
| MOTA | 577 | CG | GLU | 71 | 41.387 | | | 1.00 32.31 | AAAA |
| ATOM | 578 | CD | GLU | · 71 | 42.782 | 25.920 | 32.193 | | |
| ATOM | 579 | OE1 | GLU | 71 | 42.893 | 25.741 | 30.958 | 1.00 27.07 | AAAA |
| | | | | 71 | 43.762 | 26.117 | 32.941 | 1.00 24.85 | AAAA |
| MOTA | 580 | OE2 | | | | | | 1.00 16.48 | AAAA |
| ATOM | 581 | С | GLU | 71 | 40.580 | 28.208 | 34.466 | | |
| ATOM | . 582 | 0 | GLU | 71 | 40.831 | 29.066 | 33.611 | 1.00 17.20 | AAAA |
| | | | ALA | 72 | 39.380 | 28.097 | 35.027 | 1.00 15.68 | AAAA |
| MOTA | 583 | N | | | | | 34.644 | 1.00 16.07 | AAAA |
| MOTA | 584 | CA | ALA | 72 | 38.300 | 28.998 | | | |
| ATOM | 585 | CB | ALA | 72 | 37.035 | 28.669 | 35.425 | 1.00 17.21 | AAAA |
| | | c | ъLА | 72 | 38.678 | 30.453 | 34.897 | 1.00 19.07 | AAAA |
| ATOM | 586 | | | | | | 34.054 | 1.00 15.92 | AAAA |
| ATOM | 587 | 0 | ALA | 72 | 38.448 | 31.326 | | | |
| ATOM | 588 | N | GLU | 73 | 39.260 | 30.726 | 36.062 | 1.00 15.86 | AAAA |
| | | CA | GLU | 73 | 39.616 | 32.097 | 36.372 | 1.00 15.50 | AAAA |
| MOTA | 589 | | | | | | 37.828 | 1.00 14.12 | AAAA |
| ATOM | 590 | CB | GLU | 73 | 40.046 | 32.210 | | 1.00 14.24 | AAAA |
| ATOM | 591 | CG | GLU | 73 | 40.430 | 33.615 | 38.214 | 1.00 14.44 | |
| | | CD | GLU | 73 | 40.961 | 33.699 | 39.629 | 1.00 17.23 | AAAA |
| ATOM | 592 | | | | | | 40.573 | 1.00 18.51 | AAAA |
| MOTE | 593 | OE1 | | 73 | 40.147 | 33.696 | | 1.00 20.88 | AAAA |
| ATOM | 5 94 | OE2 | GLU | 73 | 42.201 | 33.753 | 39.793 | 1.00 40.00 | MANA |
| | | | | | | | - | | • |
| | | | | | | | | | |

28/263 Figure 16-10

| | | | CT 11 | 77 | 40.000 | | 25 425 | | |
|---------------|------------|----------|---------------|------------|------------------|------------------|------------------|--------------------------|------------------------------|
| MOTA MOTA | 595 596 | | GLU GLU | | 40.706 40.527 | | | | AAAA |
| ATOM | 597 | | | 74 | 41.832 | | | 1.00 17.74 1.00 21.57 | AAAA |
| MOTA | 598 | | | 74 | 42.911 | | | 1.00 19.48 | AAAA AAAA |
| ATOM | 599 | | | 74 | 44.256 | | | 1.00 18.48 | AAAA |
| MOTA | 600 | C | G ARG | 74 | 44.365 | | | 1.00 14.96 | AAAA |
| MOTA | 601 | CI |) ARG | 74 | 45.723 | 29.892 | 34.745 | 1.00 15.05 | AAAA |
| MOTA | 602 | | | 74 | 45.918 | | | 1.00 18.16 | AAAA |
| MOTA | 603 | | | · 74 | 46.439 | | | 1.00 16.31 | AAAA |
| ATOM | 604 | | 11 ARG | 74 | 46.843 | | | 1.00 19.74 | AAAA |
| MOTA | 605 606 | | i2 ARG ARG | 74 74 | 46.466 | | | 1.00 14.73 | AAAA |
| ATOM ATOM | 607 | | ARG | 74 | 42.643 43.148 | 32.718 33.621 | 33.084 32.426 | 1.00 16.86 | AAAA |
| ATOM | 608 | | CYS | 75 | 41.859 | 31.794 | 32.547 | 1.00 13.41 | AAAA AAAA |
| MOTA | 609 | | | 75 | 41.544 | 31.833 | 31.115 | 1.00 18.24 | AAAA |
| ATOM | 610 | | | 75 | 41.474 | 30.414 | 30.545 | 1.00 20.94 | AAAA |
| MOTA | 611 | SG | CYS | 75 | 43.047 | 29.514 | 30.572 | 1.00 19.30 | AAAA |
| MOTA | 612 | C | CYS | 75 | 40.216 | 32.561 | 30.898 | 1.00 15.81 | AAAA |
| MOTA | 613 | 0 | CYS | 75 | 39.762 | 32.748 | 29.762 | 1.00 17.79 | AAAA |
| ATOM | 614 | N | GLN | 76 | 39.601 | 32.959 | 32.007 | | AAAA |
| MOTA | 615 | CA | | 76 76 | 38.339 | 33.686 | 32.010 | 1.00 23.22 | AAAA |
| A'TOM ATOM | 616 617 | CE | | 76 76 | 38.595 37.564 | 35.122 36.107 | 31.530 32.027 | 1.00 22.99 | AAAA |
| ATOM | 618 | CD | | 76 | 37.588 | 36.229 | 33.535 | 1.00 44.69 1.00 47.78 | AAAA AAAA |
| ATOM | 619 | | 1 GLN | 76 | 37.563 | 35.228 | 34.243 | 1.00 62.95 | AAAA |
| MOTA | 620 | NE | 2 GLN | 76 | 37.619 | 37.452 | 34.033 | 1:00 45.96 | AAAA |
| MOTA | 621 | C | GLN | 76 | 37.304 | 32.975 | 31.135 | 1.00 23.43 | AAAA |
| MOTA | 622 | 0 | GLN | 76 | 36.826 | 33.512 | 30.135 | 1.00 19.93 | AAAA |
| ATOM | 623 | N | CYS | 77 | 36.951 | 31.754 | 31.521 | 1.00 15.97 | AAAA |
| MOTA MOTA | 624 625 | CA CB | CYS CYS | . 77 77 | 36.004 36.738 | 30.979 | 30.741 29.623 | 1.00 18.91 | AAAA |
| ATOM | 626 | SG | CYS | 77 | 37.848 | 30.225 28.887 | 30.269 | 1.00 24.64 1.00 25.26 | AAAA AAAA |
| ATOM | 627 | c | CYS | 77 | 35.302 | 29.951 | 31.594 | 1.00 23.28 | AAAA |
| ATOM | 628 | 0 | CYS | 7 7 | 35.685 | 29.702 | 32.732 | 1.00 20.02 | AAAA |
| MOTA | 629 | N | VAL | 78 | 34.254 | 29.366 | 31.022 | 1.00 16.00 | AAAA |
| MOTA | 630 | CA | VAL | 78 | 33.531 | 28.288 | 31.671 | 1.00 18.73 | AAAA |
| MOTA | 631 632 | CB | VAL L VAL | 78 78 | 32.016 | 28.455 | 31.557 | 1.00 15.57 | AAAA |
| ATOM ATOM | 633 | | VAL | 78 | 31.312 31.603 | 27.304 29.792 | 32.262 32.151 | 1.00 21.27 1.00 19.47 | AAAA AAAA |
| ATOM | 634 | C. | VAL | 78 | 33.950 | 27.077 | 30.859 | 1.00 19.47 | AAAA |
| ATOM | 635 | 0 | VAL | 78 | 33.499 | 26.894 | 29.718 | 1.00 24.08 | AAAA |
| MOTA | 636 | N | PRO | 79 | 34.848 | 26.249 | 31.420 | 1.00 18.91 | AAAA |
| MOTA | 637 | CD | PRO | 79 | 35.470 | 26.341 | 32.756 | 1.00 17.70 | AAAA |
| ATOM | 638 | CA | PRO. | 79 70 | 35.320 | 25.056 | 30.720 | 1.00 23.37 | AAAA |
| ATOM ATOM | 639 640 | CB | PRO PRO | 79 79 | 36.295 36.802 | 24.432 25.677 | 31.732 32.498 | 1.00 21.92 | AAAA |
| ATOM | 641 | C | PRO | 79 | 34.152 | 24.144 | 30.376 | 1.00 20.90 1.00 27.44 | A AAA A AAA |
| MOTA | 642 | ō | PRO | 79 | 33.177 | 24.064 | 31.119 | 1.00 22.20 | AAAA |
| MOTA | 643 | N | LYS | 80 | 34.245 | 23.488 | 29.224 | 1.00 23.35 | AAAA |
| MOTA | 644 | CA | LYS | 80 | 33.212 | 22.570 | 28.775 | 1.00 26.78 | AAAA |
| MOTA | 645 | CB | LYS | 80 | 33.708 | 21.853 | 27.518 | 1.00 32.33 | AAAA |
| ATOM | 646 | CG | LYS | 80 | 35.098 | 21.256 | 27.680 | 1.00 51.34 | λλλΑ |
| MOTA | 647 648 | CE. | LYS LYS | 80 80 | 35.669 37.131 | 20.817 | 26.336 26.451 | 1.00 68.70 | AAAA |
| MOTA MOTA | 649 | NZ | LYS | 80 | 37.688 | 20.401 19.949 | 25.141 | 1.00 70.04 1.00 73.72 | AAAA AAAA |
| ATOM | 650 | C | LYS | 80 | 32.875 | 21.571 | 29.875 | 1.00 73.72 | AAAA |
| ATOM | 651 | ō | LYS | 80 | 33.770 | 20.957 | 30.458 | 1.00 24.23 | AAAA |
| ATOM | 652 | N | GLY | 81 | 31.582 | 21.431 | 30.161 | 1.00 16.74 | AAAA |
| ATOM | 653 | CA | GLY | 81 | 31.126 | 20.509 | 31.194 | 1.00 18.96 | AAAA |
| MOTA | 654 | С | GLY | 81 | 31.151 | 21.039 | 32.630 | 1.00 22.38 | AAAA |
| ATOM | 655 | 0 | GLY | 81 | 30.604 | 20.396 | 33.527 | 1.00 19.29 | AAAA |
| ATOM | 656 | N | ALA | 82 | 31.754 | 22.202 | 32.863 | 1.00 22.57 | AAAA |
| MOTA | 657 658 | CA | ALA | 82 82 | 31.858 33.065 | 22.738 | 34.235 | 1.00 20.65 | AAAA |
| ATOM ATOM | 659 | CB CB | ALA ALA | 82 82 | 30.610 | 23.704 23.425 | 34.333 34.781 | 1.00 20.41 1.00 21.81 | AAAA AAAA |
| ATOM | 660 | Ö | ALA | 82 | 30.425 | 23.529 | 35.994 | 1.00 21.81 | AAAA |
| | | | | | | | | | |

| | C C 1 | NT | 300 | 83 | 29.758 | 23.926 | 33.897 | 1.00 17.68 | B AAAA |
|------|-------|-----|-------|------|--------|--------|-----------------|------------|--------|
| MOTA | 661 | N | ARG | | | | | | |
| ATOM | 662 | ÇA | ARG | 83 | 28.549 | 24.596 | 34.360 | 1.00 15.04 | |
| ATOM | 663 | CB | ARG | 83 | 27.777 | 25.188 | 33.176 | 1.00 21.02 | AAAA |
| MOTA | 664 | CG | ARG | 83 | 26.938 | 26.395 | 33.528 | 1.00 36.77 | AAAA 7 |
| | 665 | CD | ARG | 83 | 26.061 | 26.167 | 34.729 | 1.00 41.28 | |
| ATOM | | | | | | | | | |
| ATCM | 666 | NE | ARG | 83 | 25.366 | 27.393 | 35.105 | 1.00 40.05 | |
| ATOM | 667 | CZ | _ARG | 83 | 24.530 | 27.492 | 36.134 | 1.00 51.15 | 5 AAAA |
| ATOM | 668 | NH3 | L ARG | 83 | 24.286 | 26.432 | 36.893 | 1.00 55.10 |) AAAA |
| ATCM | 669 | | 2 ARG | 83 | 23.931 | 28.646 | 36.399 | 1.00 54.26 | AAAA |
| | | | | 83 | 27.701 | 23.530 | 35.030 | 1.00 21.3 | |
| ATCM | 670 | С | ARG | | | | | | |
| MOTA | 671 | 0 | ARG | 83 - | 27.193 | 23.708 | 36.130 | 1.00 24.88 | |
| ATOM | 672 | N | GLU | 84 | 27.565 | 22.406 | 34 <i>.</i> 352 | 1.00 18.76 | AAAA |
| ATOM | 673 | CA | GLU | 84 | 26.768 | 21.299 | 34.859 | 1.00 24.12 | AAAA |
| | 674 | CB | GLU | 84 | 26.527 | 20.290 | 33.744 | 1.00 32.64 | |
| MOTA | | | | | 27.769 | 19.994 | 32.925 | 1.00 37.91 | |
| MOTA | 675 | CG | GLU | 84 | | | | | |
| ATOM | 676 | CD | GLU. | 84 | 27.832 | 20.784 | 31.612 | 1.00 51.24 | |
| MOTA | 677 | OEl | GLU | 84 | 27.585 | 20.152 | 30.545 | 1.00 24.82 | AAAA . |
| MOTA | 678 | OE2 | GLU | 84 | 28.114 | 22.018 | 31.650 | 1.00 22.57 | AAAA |
| | 679 | c | GLU | 84 | 27.394 | 20.570 | 36.043 | 1.00 25.36 | |
| ATOM | | | | | | | 37.057 | 1.00 26.17 | |
| MOTA | 680 | 0 | GLU | 84 | 26.739 | 20.321 | | | |
| ATOM | 681 | N | LYS | 85 | 28.665 | 20.232 | 35.897 | 1.00 18.78 | |
| MOTA | 682 | CA | LYS | 85 | 29.399 | 19.497 | 36.915 | 1.00 20.03 | AAAA |
| ATOM | 683 | CB | LYS | 85 | 30.658 | 18.900 | 36.280 | 1.00 18.59 | AAAA |
| | 684 | CG | LYS | 85 | 31.603 | 18.223 | 37.268 | 1.00 35.69 | |
| ATOM | | | | 85 | 31.151 | 16.832 | 37.644 | 1.00 51.53 | |
| ATOM | 685 | CD | LYS | | | | | | |
| ATOM | 686 | CE | LYS | 85 | 31.451 | 15.864 | 36.520 | 1.00 59.18 | |
| ATCM | 687 | NZ | LYS | 85 | 32.914 | 15.858 | 36.240 | 1.00 56.63 | |
| ATOM | 688 | С | LYS | 85 | 29.811 | 20.263 | 38.181 | 1.00 18.33 | AAAA l |
| ATOM | 689 | 0 | LYS | 85 | 29.696 | 19.738 | 39.290 | 1.00 21.69 | AAAA |
| | 690 | N | TYR | 86 | 30.274 | 21.495 | 38.012 | 1.00 19.45 | |
| ATOM | | | | | | 22.272 | | 1.00 14.26 | |
| MOTA | 691 | CA | TYR | 86 | 30.776 | | 39.145 | | |
| ATOM | 692 | CB | TYR | 86 | 32.207 | 22.692 | 38.840 | 1.00 14.95 | |
| ATOM | 693 | CG | TYR | 86 | 33.107 | 21.508 | 38.585 | 1.00 19.76 | AAAA c |
| ATOM | 694 | CD1 | TYR | 86 . | 33.384 | 20.591 | 39.601 | 1.00 18.83 | AAAA |
| ATOM | 695 | CE1 | | 86 | 34.247 | 19.519 | 39.388 | 1.00 20.29 | AAAA (|
| | | | | 86 | 33.711 | 21.322 | 37.337 | 1.00 18.14 | |
| ATOM | 696 | CD2 | | | | | | | |
| MOTA | 697 | CE2 | | 86 | 34.567 | 20.261 | 37.112 | 1.00 22.66 | |
| ATOM | 698 | CZ | TYR | 86 | 34.832 | 19.364 | 38.145 | 1.00 22.51 | |
| MOTA | 699 | OH | TYR | 86 | 35.680 | 18.317 | 37.921 | 1.00 23.68 | AAAA |
| ATOM | 700 | С | TYR | 86 | 29.967 | 23.493 | 39.526 | 1.00 19.03 | AAAA |
| | 701 | ō | TYR | 86 | 30.353 | 24.226 | 40.450 | 1.00 19.18 | AAAA (|
| ATOM | | | | 87 | 28.873 | 23.721 | 38.803 | 1.00 17.59 | |
| ATOM | 702 | N | ASN | | | | | | |
| ATOM | 703 | CA | ASN | 87 | 27.953 | 24.843 | 39.071 | 1.00 18.07 | |
| ATOM | 704 | CB | ASN | 87 | 27.413 | 24.730 | 40.514 | 1.00 23.87 | |
| ATOM | 705 | CG | ASN | 87 | 26.020 | 25.349 | 40.688 | 1.00 30.67 | AAAA: |
| ATOM | 706 | OD1 | ASN | 87 | 25.531 | 25.520 | 41.819 | 1.00 31.55 | AAAA c |
| | 707 | | ASN | 87 | 25.370 | 25.661 | 39.580 | 1.00 20.18 | AAAA 8 |
| ATOM | | | ASN | · 87 | 28.641 | 26.197 | 38.875 | 1.00 24.24 | |
| ATOM | 708 | C | | | | | | | |
| ATOM | 709 | 0 | ASN | 87 | 28.283 | 27.190 | 39.519 | 1.00 18.57 | |
| ATCM | 710 | N | ILE | 88 | 29.617 | 26.237 | 37.970 | 1.00 18.80 | |
| MOTA | 711 | CA | ILE | 88 | 30.353 | 27.471 | 37.680 | 1.00 18.55 | AAAA |
| | 712 | CB | ILE | 88 | 31.865 | 27.166 | 37.508 | 1.00 26.44 | AAAA |
| MOTA | | | ILE | 88 | 32.613 | 28.406 | 37.044 | 1.00 43.71 | |
| ATCM | 713 | | | | | | | 1.00 36.30 | |
| atcm | .714 | CG1 | ILE | 88 | 32.439 | 26.703 | 38.835 | | |
| MOTA | 715 | CD1 | ILE | 88 | 32.295 | 27.735 | 39.888 | 1.00 24.08 | |
| ATOM | 716 | С | ILE | 88 | 29.887 | 28.142 | 36.392 | 1.00 14.36 | AAAA |
| | 717 | 0 | ILE | 88 | 29.584 | 27.459 | 35.426 | 1.00 21.93 | AAAA |
| ATOM | | | | 89 | 29.843 | 29.473 | 36.380 | 1.00 18.73 | |
| ATCM | 718 | И | GLY | | | | | 1.00 20.23 | |
| ATOM | 719 | CA | GLY | 89 | 29.479 | 30.162 | 35.154 | | |
| ATOM | 720 | C | GLY | 89 | 28.147 | 30.873 | 35.106 | 1.00 20.85 | AAAA |
| ATCM | 721 | 0 | GLY | 89 | 28.006 | 31.817 | 34.330 | 1.00 25.47 | |
| | 722 | N | GLY | 90 | 27.172 | 30.414 | 35.889 | 1.00 21.17 | |
| ATCM | | | GLY | 90 | 25.863 | 31.060 | 35.898 | 1.00 24.44 | |
| ATOM | 723 | CA | | | | | | 1.00 30.60 | |
| ATOM | 724 | C | GLY | 90 | 25.862 | 32.371 | 36.668 | | |
| ATCM | 725 | 0 | GLY | 90 | 26.900 | 32.788 | 37.168 | 1.00 28.13 | AAAA |
| ATCM | 726 | N | TYR | 91 | 24.708 | 33.036 | 36.755 | 1.00 23.38 | AAAA |
| | | | | | | | - | | • |

| ATOM | | CA TYR | 91 | 24.59 | | 9 37.490 | 1.00 28.48 | 2222 |
|--------------|-----------------|--------------|----------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | | CB TYR | 91 | 23.14 | 4 34.75 | | 1.00 29.88 | AAAA |
| ATOM | | CG TYR | 91 | 22.92 | | | | AAAA |
| ATOM | | CD1 TYR | | 23.32 | 9 37.19 | | | AAAA |
| MOTA | | CE1 TYR | 91 | 23.13 | 0 38.25 | | 1.00 31.76 | AAAA AAAA |
| ATOM- | | CD2 TYR | 91 | 22.31 | 7 35.67 | | | AAAA |
| MOTA | | CE2 TYR | 91 | 22.11 | | 40.664 | | |
| MOTA | 734 (| CZ TYR | 91 | 22.52 | | | | AAAA |
| ATOM | 735 | OH TYR | 91 | 22.30 | | | | AAAA |
| ATOM | 736 (| TYR | 91 | 25.07 | | 38.937 | | AAAA |
| ATOM | 737 (| TYR | 91 | 25.713 | | 39.502 | | AAAA |
| ATOM | 738 N | I GLU | 92 | 24.724 | 33.032 | | | AAAA |
| ATOM | 739 C | A GLU | 92 | 25.048 | | | | AAAA |
| MOTA | 740 C | B GLU | 92 | 24.289 | | | | AAAA |
| MOTA | 741 C | G GLU | 92 | 24.595 | | | 1.00 41.38 | AAAA |
| ATOM | 742 C | D GLU | 92 | 23.604 | | | | AAAA |
| ATOM | 743 O | E1 GLU | 92 | 24.008 | | | 1.00 45.51 | - AAAA |
| ATOM | 744 O | E2 GLU | 92 | 22.418 | | | 1.00 38.16 | AAAA |
| MOTA | 745 C | GLU | 92 | 26.541 | | | 1.00 25.78 | AAAA |
| ATOM | 746 o | GLU | 92 | 27.045 | | | 1.00 24.95 | AAAA |
| MOTA | 747 N | ASN | 93 | 27.243 | | | 1.00 21.41 | AAAA |
| ATOM | 748 C. | A ASN | 93 | 28.674 | | | 1.00 21.14 | AAAA AAAA |
| ATOM | 749 C | B ASN | 93 | 28.876 | 30.075 | | 1.00 17.27 | AAAA |
| ATOM | 750 C | | 93 | 27.905 | 29.682 | 42.320 | 1.00 15.34 | AAAA |
| ATOM | | D1 ASN | 93 | 27.882 | 30.290 | 43.399 | 1.00 20.33 | AAAA |
| ATOM | | D2 ASN | 93 | 27.078 | 28.674 | 42.047 | 1.00 20.49 | AAAA |
| MOTA | 753 C | ásn | 93 | 29.378 | 31.778 | 39.445 | 1.00 22.25 | AAAA |
| ATOM | 754 0 | ASN | 93 | 29.901 | 30.865 | 38.806 | 1.00 20.29 | AAAA |
| MOTA | 755 N | PRO | 94 | 29.451 | 33.057 | 39.045 | 1.00 25.45 | AAAA |
| ATOM | 756 CI | | 94 | 29.027 | 34.221 | 39.839 | 1.00 23.03 | AAAA |
| MOTA | 757 CA | | 94 | 30.055 | 33.523 | 37.794 | 1.00 23.05 | AAAA |
| MOTA | 758 CE | | 94 | 29.669 | 35.004 | 37.759 | 1.00 28.71 | AAAA |
| ATOM | 759 CG | | 94 | 28.528 | 35.112 | . 38.755 | 1.00 40.02 | AAAA |
| ATOM | 760 C | PRO | 94 | 31.554 | 33.384 | 37.697 | 1.00 26.51 | AAAA |
| ATOM | 761 O 762 N | PRO | 94 | 32.232 | 33.185 | 38.688 | 1.00 17.36 | AAAA |
| ATOM ATOM | 762 N 763 CA | VAL | 95 05 | 32.068 | 33.498 | 36.478 | 1.00 21.12 | AAAA |
| ATOM | 764 CB | | 95 05 | 33.506 | 33.493 | 36.281 | 1.00 17.00 | AAAA |
| ATOM | | VAL 1 VAL | 95 95 | 33.851 | 33.242 | 34.796 | 1.00 25.15 | AAAA |
| ATOM | | 2 VAL | 95 95 | 35.326 | 33.537 | 34.533 | 1.00 27.19 | AAAA |
| ATOM | 767 C | VAL | 95 | 33.551 | 31.791 | 34.443 | 1.00 17.37 | AAAA |
| ATOM | 768 0 | VAL | 95 | 33.989 33.426 | 34.899 | 36.686 | 1.00 17.42 | AAAA |
| ATOM | 769 ม | SER | 96 | 34.986 | 35.894 | 36.237 | 1.00 23.43 | AAAA |
| ATOM | 770 CA | SER | 96 | 35.564 | 34.982 | 37.563 | 1.00 18.84 | AAAA |
| ATOM | 771 CB | SER | 96 | 34.608 | 36.270 37.070 | 37.982 38.867 | 1.00 21.77 | AAAA |
| ATOM | 772 OG | SER | 96 | 34.723 | 36.679 | 40.223 | 1.00 23.11 | AAAA |
| ATOM | 773 C | SER | 96 | 36.835 | 35.987 | 38.789 | 1.00 24.43 1.00 29.09 | AAAA |
| ATCM | 774 O | SER | 96 . | 37.117 | 34.828 | 39.115 | 1.00 27.12 | AAAA |
| MOTA | 775 N | TYR | 97 | 37.610 | 37.020 | 39.124 | 1.00 27.12 | AAAA |
| MOTA | 776 CA | TYR | | 38.803 | 36.751 | 39.911 | 1.00 20.69 | AAAA AAAA |
| MOTA | 777 CB | TYR | 97 | 39.865 | 37.835 | 39.712 | 1.00 21.82 | AAAA |
| ATOM | 778 CG | TYR | 97 | 40.492 | 37.748 | 38.332 | 1.00 22.72 | AAAA |
| ATOM | 779 CD1 | TYR | 97 | 39.936 | 38.414 | 37.235 | 1.00 28.47 | AAAA |
| ATOM | 780 CE1 | TYR | 97 | 40.473 | 38.265 | 35.949 | 1.00 24.45 | AAAA |
| ATOM | 781 CD2 | TYR | 97 | 41.599 | 36.929 | 38.112 | 1.00 19.74 | AAAA |
| ATOM | 782 CE2 | | 97 | 42.144 | 36.771 | 36.832 | 1.00 21.63 | AAAA |
| ATOM | 783 CZ | TYR | 97 | 41.578 | 37.439 | 35.759 | 1.00 23.13 | AAAA |
| ATOM | 784 OH | TYR | 97 | 42.122 | 37.273 | 34.501 | 1.00 28.54 | AAAA |
| ATOM | 785 C | TYR | 97 | 38.510 | 36.515 | 41.393 | 1.00 20.12 | AAAA |
| ATOM | 786 O | TYR | 97 | 39.413 | 36.285 | | 1.00 19.76 | AAAA |
| MOTA | 787 N | ALA | 98 | 37.243 | 36.558 | 4.4 | 1.00 18.56 | AAAA |
| ATOM | 788 CA | ALA | 98 | | 36.259 | | 1.00 22.23 | AAAA |
| ATOM | 789 CB | ALA | 98 | | 36.888 | | 1.00 27.92 | AAAA |
| ATOM · | 790 C | ALA | 98 | 36.776 | | | 1.00 23.56 | AAAA |
| MOTA | 791 O | ALA | 98 | | 34.166 | | 1.00 20.14 | AAAA |
| MOTA | 792 N | MET | 99 | | | | 1.00 16.84 | AAAA |
| • | | | _ | | | | | |

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| ATOM | 793 | | | | 36.295 | 32.643 | 42.117 | 1.00 17.60 | AAAA |
|--------------|------------|------------|----------------|------------|-------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 794 | | - | | 35.864 | 32.137 | 40.736 | 1.00 17.05 | AAAA |
| ATOM | 795 | | | | 36.999 | 31.824 | 39.793 | 1.00 11.16 | AAAA |
| ATOM | 796 797 | | | | 36.314 35.165 | 31.698 30.295 | 38.113 38.312 | 1.00 16.54 1.00 17.83 | AAAA |
| ATOM ATOM | 798 | | MET | | 37.432 | 31.800 | 42.650 | 1.00 17.83 | AAAA AAAA |
| ATOM | 799 | | MET | | 37.197 | 30.753 | 43.251 | 1.00 18.21 | AAAA |
| ATOM | . 800 | | PHE | | 38.670 | 32.216 | 42.420 | 1.00 12.87 | AAAA |
| MOTA | 801 | CA | PHE | 100 | 39.774 | 31.439 | 42.987 | 1.00 17.13 | AAAA |
| MOTA | 802 | CB | | | 40.559 | 30.681 | 41.917 | 1.00 15.23 | AAAA |
| ATOM | 803 | CG | | | 41.647 | 29.834 | 42.492 | 1.00 15.20 | AAAA |
| MOTA MOTA | 804 805 | | 1 PHE 2 PHE | 100 100 | 41.342 42.972 | 28.638 30.282 | 43.140 42.488 | 1.00 22.96 1.00 17.12 | AAAA |
| ATOM | 806 | | 1 PHE | 100 | 42:341 | 27.901 | 43.782 | 1.00 17.12 | AAAA AAAA |
| ATOM | 807 | | 2 PHE | 100 | 43.974 | 29.552 | 43.129 | 1.00 16.99 | AAAA |
| ATOM | 808 | CZ | PHE | 100 | 43.658 | 28.360 | 43.779 | 1.00 17.78 | AAAA |
| MOTA | 809 | С | PHE | 100 | 40.755 | 32.305 | 43.774 | 1.00 20.54 | AAAA |
| MOTA | 810 | 0 | PHE | 100 | 41.088 | 31.990 | 44.912 | 1.00 21.45 | AAAA |
| MOTA | 811 812 | N CA | THR THR | 101 101 | 41.219 | 33.401 34.245 | 43.187 43.902 | 1.00 18.02 1.00 15.25 | AAAA |
| MOTA MOTA | 813 | CB | THR | 101 | 42.715 | 35.341 | 42.976 | 1.00 15.25 | AAAA AAAA |
| MOTA | 814 | | 1 THR | 101 | 43.386 | 34.720 | 41.870 | 1.00 16.01 | AAAA |
| ATOM | 815 | CG | 2 THR | 101 | 43.706 | 36.226 | 43.697 | 1.00 16.31 | AAAA |
| ATOM | 816 | C | THR | 101 | 41.567 | 34.860 | 45.160 | 1.00 14.12 | AAAA |
| MOTA | 817 | O N | THR GLY | 101 102 | 42.110 40.435 | 34.707 35.541 | 46.244 | 1.00 16.86 | AAAA |
| ATOM ATOM | 818 819 | N CA | GLY | 102 | 39.770 | 36.145 | 45.008 46.156 | 1.00 13.77 1.00 16.29 | AAAA AAAA |
| ATOM | 820 | C | GLY | 102 | 39.330 | 35.065 | 47.133 | 1.00 16.75 | AAAA |
| MOTA | 821 | 0 | GĹY | 102 | 39.502 | 35.202 | 48.338 | 1.00 14.48 | AÄAA |
| ATOM | 822 | N | SER | 103 | 38.752 | 33.986 | 46.615 | 1.00 16.24 | AAAA |
| MOTA | 823 | CA | SER | 103 | 38.315 | 32.890 | 47.488 | 1.00 16.72 | AAAA |
| ATOM ATOM | 824 825 | CB OG | SER SER | 103 103 | 37.567 36.339 | 31.821 32.349 | 46.684 46.197 | 1.00 15.97 1.00 26.86 | AAAA AAAA |
| ATOM | 826 | c | SER | 103 | 39.494 | 32.264 | 48.218 | 1.00 17.88 | AAAA |
| ATOM | 827 | 0 | SER | 103 | 39.405 | 31.974 | 49.419 | 1.00 14.17 | AAAA |
| ATOM | 828 | N | SER | 104 | 40.604 | 32.057 | 47.515 | 1.00 11.40 | AAAA |
| ATOM | 829 | CA | SER | 104 | 41.780 | 31.484 | 48.181 | 1.00 17.61 | AAAA |
| ATOM ATOM | 830 831 | CB OG | SER SER | 104 104 | 42.888 42.525 | 31.206 30.102 | 47.160 46.362 | 1.00 15.89 1.00 27.82 | AAAA AAAA |
| ATOM | 832 | c | SER | 104 | 42.332 | 32.404 | 49.271 | 1.00 17.02 | AAAA |
| ATOM | 833 | 0 | SER | 104 | 42.867 | 31.958 | 50.286 | 1.00 15.37 | AAAA |
| ATOM | 834 | N | LEU | 105 | 42.206 | 33.698 | 49.052 | 1.00 17.10 | AAAA |
| ATOM | 835 | CA | LEU | 105 | 42.709 | 34.652 | 50.016 | 1.00 16.95 | AAAA |
| ATOM | 836 837 | CB - | LEU | 105 105 | 42.728 43.613 | 36.037 37.108 | 49.365 49.981 | 1.00 18.44 1.00 29.88 | AAAA AAAA |
| ATOM ATOM | 838 | | LEU | 105 | 45.086 | 36 631 | 49.959 | 1.00 20.25 | AAAA |
| ATOM | 839 | | LEU | 105 | 43.438 | 38 418 | 49.175 | 1.00 29.39 | AAAA |
| ATOM | 840 | С | LEU | 105 | 41.837 | 34 637 | 51.282 | 1.00 14.81 | AAAA |
| ATOM | 841 | 0 | LEU | 105 | 42.334 | 34.703 | 52.404 | 1.00 17.74 | AAAA |
| ATOM | 842 | N | ALA | 106 | 40.532 | 34.531 | 51.095 | 1.00 19.28 | AAAA |
| ATOM ATOM | 843 844 | CA CB | ALA ALA | 106 106 | 39.601 38.140 | 34.493 34.574 | 52.224 51.704 | 1.00 12.39 1.00 11.58 | AAAA AAAA |
| ATOM | 845 | c | ALA | 106 | 39.807 | 33.210 | 53.023 | 1.00 14.79 | AAAA |
| ATOM | 846 | 0 | ALA | 106 | 39.704 | 33.203 | 54.250 | 1.00 13.58 | AAAA |
| ATOM | 847 | N | THR | 107 | 40.114 | 32.128 | 52.318 | 1.00 13.67 | AAAA |
| MOTA | 848 | CA | THR | 107 | 40.314 | 30.819 | 52.956 | 1.00 13.21 | AAAA |
| ATOM | 849 050 | CB | THR THR | 107 107 | 40.187 38.868 | 29.708 | 51.902 | 1.00 14.95 1.00 15.72 | AAAA AAAA |
| MOTA MOTA | 850 851 | OG1 CG2 | | 107 | 40.422 | 29.792 28.311 | 51.334 52.511 | 1.00 13.72 | AAAA |
| ATOM | 852 | C | THR | 107 | 41.649 | 30.751 | 53.687 | 1.00 15.80 | AAAA |
| ATOM | 853 | 0 | THR | 107 | 41.734 | 30.206 | 54.792 | 1.00 15.63 | AAAA |
| ATOM | 854 | | GLY | 108 | 42.696 | 31.294 | 53.082 | 1.00 14.08 | AAAA |
| ATOM | 855 | CA | GLY | 108 | 43.968 | 31.298 | 53.765 | 1.00 14.62 | AAAA |
| ATOM · | 856 057 | Ċ | GLY GLY | 108 108 | 43.801. 44.417 | 32.119 | 55.041 | 1.00 20.05 1.00 17.53 | AAAA AAAA |
| ATOM ATOM | 857 858 | O N | SER | 109 | 42.963 | 31.813 33.158 | 56.063 54.988 | 1.00 17.33 | AAAA |
| ALCH | 0.50 | ٠. | | | | JJ.136 | - | | |
| | | | | | | | | | |

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| ATOM | 859 CA S | ER 109 | 40 70 | | | | |
|--------|--------------|--------|---------|----------|----------------|-------------|--------|
| | | | 42.72 | | | | AAAA |
| ATOM | | ER 109 | 41.90 | 6 35.248 | 3 55.737 | 1.00 15.58 | |
| ATOM | 861 OG 5 | ER 109 | 42.62 | | | | AAAA |
| ATOM | | ER 109 | | 7 30.043 | 54.809 | | . AAAA |
| | | | 42.03 | | 57.297 | 1.00 15.56 | AAAA |
| MOTA | 863 O SI | ER 109 | 42.18 | 9 33.600 | | | |
| ATOM | 864 N T | HR 110 | 41.26 | | | | AAAA |
| ATOM | | | | | | | AAAA |
| | | HR 110 | 40.60 | | 57.957 | 1.00 12.89 | AAAA |
| ATOM | 866 CB TI | IR 110 | 39.45 | 2 30.628 | | 1 00 14 54 | |
| MOTA | 867 OG1 TE | | | _ | | | AAAA |
| | | | 38.34 | | 57.163 | 1.00 18.11 | AAAA |
| ATOM | . 868 CG2 TF | IR 110 | 39.06 | 1 29.452 | 58.278 | 1.00 12.91 | |
| MOTA | 869 C TH | IR 110 | 41.63 | | | 1.00 12.91 | AAAA |
| MOTA | | | | | | 1.00 18.44 | AAAA |
| | | | 41.574 | 4 30.302 | 59.806 | 1.00 16.30 | AAAA |
| ATOM | 871 N VA | L 111 | 42.584 | 4 30.013 | | | |
| ATOM | 872 CA VA | L 111 | 43.614 | | | 1.00 15.20 | AAAA |
| | | | | | | 1.00 20.45 | AAAA |
| MOTA | | | 44.517 | 7 28.514 | 57.323 | 1.00 20.02 | |
| ATOM | 874 CG1 VA | L 111 | 45.652 | 27.765 | | | AAAA |
| ATOM | 875 CG2 VA | | | | | 1.00 21.79 | AAAA |
| | | | 43.697 | | 56.482 | 1.00 19.07 | AAAA |
| MOTA | 876 C VA | L 111 | 44.456 | 30.075 | | 1.00 18.21 | |
| ATOM | 877 O VA | L 111 | 44.838 | | | | AAAA |
| . ATOM | | _ | | | 60.431 | 1.00 18.65 | AAAA |
| | 878 N GL | | 44.731 | 31.302 | 58.890 | 1.00 16.82 | AAAA |
| ATOM | 879 CA GL | N 112 | 45.493 | | 59.719 | | |
| ATOM | 880 CB GL | | | | | 1.00 20.13 | AAAA |
| | | | 45.751 | | 58.970 | 1.00 22.39 | AAAA |
| ATOM | 881 CG GLI | N 112 | 46.593 | 33.360 | 57.723 | 1.00 21.17 | 1000 |
| ATOM | 882 CD GLI | N 112 | 46.797 | | 57.723 | | AAAA |
| MOTA | 883 OE1 GL | | | | 56.982 | 1.00 24.82 | AAAA |
| | | | 47.772 | 35.381 | 57.219 | 1.00 25.62 | AAAA |
| ATOM | 884 NE2 GLI | V 112 | 45.866 | | 56.091 | | |
| ATOM | 885 C GL | V 112 | 44.743 | | | 1.00 13.16 | AAAA |
| ATOM | | | | | 61.012 | 1.00 23.99 | AAAA |
| | | | 45.340 | 32.593 | 62.079 | 1.00 17.94 | AAAA |
| ATOM | 887 N ALA | 113 | 43.431 | 32.700 | 60.924 | | |
| ATOM | 888 CA ALA | 113 | | 52.700 | | 1.00 15.60 | AAAA |
| | | | 42.003 | 32.941 | 62.138 | 1.00 15.04 | AAAA |
| ATOM | 889 CB ALA | 113 | 41.191 | 33.138 | 61.802 | 1.00 18.65 | |
| ATOM | 890 C ALA | 113 | 42.807 | 31.751 | | | AAAA |
| ATOM | 891 O ALA | | | 34.73. | 63.083 | 1.00 14.84 | AAAA |
| | | | 42.941 | 31.909 | 64.296 | 1.00 21.05 | AAAA |
| MOTA | 892 N ILE | 114 | 42.767 | 30.550 | 62.534 | 1.00 16.45 | |
| ATOM | 893 CA ILE | 114 | 42.919 | | | 1.00 10.45 | AAAA · |
| ATOM | 894 CB ILE | | | 29.383 | 63.389 | 1.00 15.38 | AAAA |
| | | , | 42.600 | 28.100 | 62.637 | 1.00 15.22 | AAAA |
| ATOM | 895 CG2 ILE | 114 | 42.888 | 26.893 | 63.537 | 1.00 15.72 | |
| ATOM | 896 CG1 ILE | 114 | 41.110 | | | | AAAA |
| ATOM | | | 41.110 | 28.112 | 62.244 | 1.00 19.28 | AAAA |
| | | | 40.744 | 27.038 | 61.191 | 1.00 13.43 | AAAA |
| ATOM | . 898 C ILE | 114 | 44.329 | 29.318 | 63.968 | | |
| ATOM | 899 O ILE | 114 | | | | 1.00 18.02 | AAAA |
| | | | 44.508 | 28.998 | 65. 156 | 1.00 20.38 | AAAA |
| ATOM | 900 N GLU | 115 | 45.328 | 29.629 | 63.144 | 1.00 15.27 | |
| ATOM | 901 CA GLU | 115 | 46.726 | 29.625 | | 1.00 15.27 | AAAA |
| ATOM | 902 CB GLU | 115 | | | | 1.00 21.48 | AAAA |
| | | | 47.690 | 30.080 | 62.506 | 1.00 21.76 | AAAA |
| ATOM | 903 CG GLU | 115 | 47.884 | 29.080 | | 1.00 15.78 | |
| A.OM | 904 CD GLU | 115 | .48.670 | | | | AAAA |
| A COM | | | | 29.648 | 60.211 | 1.00 20.04 | AAAA |
| | | 115 | 49.051 | 30.843 | 60.239 | 1.00 21.48 | AAAA |
| A'1'OM | 906 OE2 GLU | 115 | 48.901 | 28.902 | | | |
| ATOM | 907 C GLU | 115 | | | | 1.00 26.59 | AAAA |
| | | | 46.877 | 30.559 | 64.814 | 1.00 23.55 | AAAA |
| MOTA | 908 O GLU | 115 | 47.509 | 30.212 | | 1.00 23.03 | |
| ATOM | 909 N GLU | 116 | 46.295 | 31 740 | | 1.00 25.05. | AAAA |
| ATOM | | | | 31.748 | | 1.00 22.73 | AAAA |
| | | 116 | 46.367 | 32.735 | 65.774 | 1.00 20.54 | AAAA |
| ATOM | 911 CB GLU | 116 | 45.744 | | 65 330 | 1.00 10 40 | |
| MOTA | .912 CG GLU | 116 | | • • | 65.320 | 1.00 18.40 | AAAA |
| | | | 46.562 | 34.765 | 64.279 | 1.00 19.76 | AAAA |
| MOTA | 913 CD GLU | 116 | 47.985 | 34.998 | | 1.00 27.24 | |
| ATOM | 914 OE1 GLU | 116 | 48.164 | | | | AAAA |
| | | | | 35.630 | 65.815 | 1.00 18.44 | AAAA |
| ATOM | 915 CE2 GLU | 116 | 48.919 | 34.543 | 64.078 1 | 1.00 23.17 | AAAA |
| ATOM | 916 C GLU | 116 | 45.682 | | | | |
| ATOM | 917 0 GLU | 116 | | 20 42= | | 1.00 25.39 | AAAA |
| | | | 46.207 | 32.427 | 68.137 1 | .00 22.87 | AAAA |
| ATOM | 918 N PHE | 117 | 44.510 | | | .00 18.78 | |
| ATOM | 919 CA PHE | 117 | | 31 120 | | | AAAA |
| | | | | | 68.019 1 | .00 22.11 | AAAA |
| MOTA | 920 CB PHE | 117 | 42.451 | 30.530 | | .00 23.14 | AAAA |
| ATOM | 921 CG PHE | 117 | | | | | |
| ATOM | | | | | 68.728 1 | .00 24.06 | AAAA |
| | | 117 | 40.880 | 30.961 6 | 69.493 1 | .00 19.67 | AAAA |
| ATOM | 923 CD2 PHE | 117 | | | | | |
| ATOM | 924 CE1 PHE | 117 | | -0./U1 C | 77.000 1 | .00 24.08 | AAAA |
| | 131 CEI PRE | TT / | 40.115 | 30.531 7 | 70.586 1 | .00 23.68 | AAAA |
| • | • | | | - | | | |

33/263 Figure 16-15

| | • | | | | | | |
|--------|-------------|---------|----------|----------|--------|------------|--------------|
| ATOM | 925 CE2 | PHE 117 | 40.799 | 28.262 | 70.156 | 1.00 24.04 | Aaaa |
| MOTA | 926 CZ | PHE 117 | 40.078 | 3 29.179 | | | |
| ATOM | 927 C | PHE 117 | 44.587 | | | | AAAA |
| ATOM | 928 O | PHE 117 | | | | | AAAA |
| ATOM | | | 44.613 | | | | AAAA |
| | | LEU 118 | 45.238 | | | 1.00 21.09 | AAAA |
| MOTA | | LEU 118 | 46.025 | 28.113 | 68.549 | 1.00 20.73 | AAAA |
| MOTA | 931. CB | LEU 118 | 46.358 | 27.075 | 67.480 | | AAAA |
| ATOM | 932 CG | LEU 118 | 45.148 | | | 1.00 26.20 | |
| ATOM | 933 CD1 | | 45.591 | | | | AAAA |
| ATOM | 934 CD2 | | | | | 1.00 34.23 | AAAA |
| | | | 44.520 | | | 1.00 27.16 | AAAA |
| MOTA | | LEU 118 | - 47.290 | 28.601 | 69.238 | 1.00 26.49 | AAAA |
| ATOM | | LEU 118 | 47.908 | 27.856 | 69.996 | 1.00 26.34 | AAAA |
| MOTA | 937 N : | LYS 119 | 47.672 | 29.848 | | 1.00 28.92 | AAAA |
| MOTA | 938 CA : | LYS 119 | 48.835 | | | 1.00 28.53 | |
| ATOM | | LYS 119 | 49.392 | | | 1.00 28.53 | AAAA |
| ATOM | | | | | | 1.00 30.15 | AAAA |
| | | LYS 119 | 49.915 | | | | · AAAA |
| ATOM | | LYS 119 | 50.291 | 32.549 | 66.716 | 1.00 28.98 | AAAA |
| MOTA | 942 CE 1 | LYS 119 | 50.905 | 32.262 | 65.380 | 1.00 31.07 | AAAA |
| ATOM | 943 NZ I | LYS 119 | 51.195 | | 64.745 | 1.00 22.46 | |
| ATOM | | LYS 119 | 48.335 | 31.053 | | | AAAA |
| ATOM | | | | | 70.932 | 1.00 35.74 | AAAA |
| | | - | 49.117 | 31.541 | 71.750 | 1.00 27.10 | AAAA |
| MOTA | | LY 120 | 47.018 | 31.050 | 71.103 | 1.00 25.20 | AAAA |
| MOTA | | SLY 120 | 46.445 | 31,605 | 72.309 | 1.00 30.18 | AAAA |
| ATOM | 948 C G | LY 120 | 45.913 | 33.007 | 72.122 | 1.00 31.91 | AAAA |
| MOTA | 949 O G | LY 120 | 45.540 | 33.665 | 73.094 | 1.00 34.76 | |
| ATOM | | SN 121 | 45.889 | 33.495 | 70.887 | 1 00 34.76 | AAAA |
| ATOM | | SN 121 | | | | 1.00 20.56 | AAAA |
| | | | 45.353 | 34.825 | 70.681 | 1.00 25.58 | AAAA |
| ATOM | | SN 121 | 46.278 | 35.634 | 69.785 | 1.00 29.99 | AAAA |
| ATOM | | SN 121 | 47.641 | 35.827 | 70.427 | 1.00-24.43 | AAAA |
| ATOM - | 954 OD1 A | | 48.396 | 34.874 | 70.588 | 1.00 54.63 | AAAA |
| MOTA | 955 ND2 A | SN 121 | 47.944 | 37.045 | 70.817 | 1.00 41.69 | AAAA |
| MOTA | 956 C A | SN 121 | 43.941 | 34.759 | 70.135 | 1.00 18.85 | |
| ATOM | | SN 121 | 43.421 | 33.675 | | | AAAA |
| ATOM | | AL 122 | | | 69.899 | 1.00 24.77 | AAAA |
| | | | 43.310 | 35.918 | 69.991 | 1.00 19.55 | AAAA |
| ATOM | | AL 122 | 41.936 | 35.994 | 69.499 | 1.00 22.90 | AAAA |
| ATOM | | AL 122 | 41.053 | 36.832 | 70.449 | 1.00 31.47 | AAAA |
| ATOM | 961 CG1 V | | 39.649 | 37.006 | 69.851 | 1.00 31.52 | AAAA |
| ATOM | 962 CG2 V | AL 122 | 40.986 | 36.154 | 71.810 | 1.00 32.50 | AAAA |
| ATOM | 963 C V | AL 122 | 41.953 | 36.632 | 68.130 | 1.00 16.87 | |
| ATOM | | AL 122 | 42.518 | 37.710 | | | AAAA |
| ATOM | | LA 123 | | | 67.938 | 1.00 24.08 | AAAA |
| | | | 41.321 | 35.983 | 67.159 | 1.00 18.67 | AAAA |
| ATOM | | LA 123 | 41.360 | 36.532 | 65.821 | 1.00 10.18 | AAAA |
| ATOM | | LA 123 | 42.346 | 35.743 | 64.990 | 1.00 19.04 | AAAA |
| ATOM | 968 C AI | LA 123 | 40.000 | 36.551 | 65.131 | 1.00 13.72 | AAAA |
| MOTA | 969 O AI | LA 123 | 39.108 | 35.761 | 65.439 | 1.00 20.78 | AAAA |
| ATOM | 970 N PE | | 39.871 | 37.457 | 64.180 | | |
| ATOM | 971 CA PH | | 38.649 | 37.610 | | 1.00 12.92 | AAAA |
| ATOM | 972 CB PH | | | | 63.401 | 1.00 14.67 | AAAA |
| | | | 37.904 | 38.878 | 63.85€ | 1.00 14.67 | AAAA |
| MOTA | 973 CG PH | | 36.660 | 39.209 | 63.049 | 1.00 20.28 | AAAA |
| ATOM | 974 CD1 PH | | 35.811 | 38.209 | 62.587 | 1.00 18.56 | AAAA |
| ATOM | 975 CD2 PH | E 124 | 36.286 | 40.545 | 62.843 | 1.00 19.53 | AAAA |
| MOTA | 976 CE1 PH | E 124 | 34.609 | 38.532 | 61.937 | 1.00 18.75 | |
| ATOM | 977 CE2 PH | | 35.072 | 40.875 | | | AAAA |
| | | | | | 62.193 | 1.00 20.18 | AAAA |
| ATOM | | | 34.242 | | 61.744 | 1.00 21.57 | AAAA |
| ATOM | 979 C PH | | 39.016 | 37.712 | 61.930 | 1.00 22.60 | AAAA |
| MOTA | 980 O PH | E 124 | 39.823 | 38.558 | 61.535 | 1.00 19.22 | AAAA |
| ATOM | 981 N AS | N 125 | 38.449 | 36.820 | 61.126 | 1.00 19.39 | AAAA |
| ATOM | 982 CA ASI | | 38.651 | 36.858 | 59.691 | | |
| ATOM | 983 CB ASI | | 39.122 | | | 1.00 16.80 | AAAA |
| | | | | 35.507 | 59.150 | 1.00 15.71 | AAA A |
| ATOM | 984 CG ASI | | 39.063 | 35.469 | 57.649 | 1.00 12.84 | AAAA |
| ATOM | 985 OD1 ASI | | 39.216 | 36.508 | 57.006 | 1.00 14.91 | AAAA |
| ATOM | 986 ND2 ASI | N 125 | 38.853 | 34.272 | 57.065 | 1.00 16.21 | AAAA |
| ATCM | 987 C ASI | N 125 | | | 59.038 | 1.00 16.22 | AAAA |
| ATOM | 988 O ASI | | 36.502 | 36.330 | | | |
| ATOM | 989 N PRO | | | | | 1.00 15.28 | AAAA |
| | | | | 38.502 | | 1.00 14.84 | AAAA |
| ATOM | 990 CD PRO | 126 | 37.908 | 39.684 | 59.052 | 1.00 18.10 | AAAA |
| • | • | | | | | | • |

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| | | | | | | | | | • | | |
|--------------|--------------|------------|------------|------------|----|-------------------------|------------------|------------------|-------|----------------------|--------------|
| ATOM | |)1 C | | | | 35.81 | 1 38.91 | 0 58.15 | 6 1.0 | 00 17.33 | AAAA |
| ATOM | | | | | | 35.91 | | | 7 1.0 | 0 16.32 | АААА |
| ATOM | | | | | | 37.41 | | | | 0 20.95 | AAAA |
| MOTA MOTA | | | PRC PRC | | | 35.54 | | | | 0 13.78 | AAAA |
| ATOM | | | | | | 34.40 | | | | 0 17.03 | AAAA |
| ATOM | | | | | | 36.60 36.46 | | | | 0 14.57 | AAAA |
| ATOM | | | | | | 37.81 | | | | 00 17.37 00 14.48 | AAAA |
| ATOM | 99 | 9 C | ALA | | | 35.98 | | | | 0 14.48 | AAAA |
| ATOM | | | ALA | | | 35.49 | | | | 0 15.62 | AAAA AAAA |
| MOTA | | | GLY | | | 36.11 | 1 35.33 | | | 0 13.54 | AAAA |
| ATOM | 100 | _ | | | _ | 35.72 | | 9 55.97. | 1.0 | 0 13.53 | AAAA |
| ATOM | 100 | _ | GLY | | | 34.234 | | | 1.0 | 0 14.49 | AAAA |
| MOTA MOTA | 100 100 | | GLY | _ | | 33.414 | | | 1.0 | 0 15.65 | AAAA |
| ATOM | 100 | | GLY GLY | 129 129 | | 33.883 | | | | 0 13.35 | AAAA |
| ATOM | 100 | | GLY | 129 | | 32.487 31.754 | | | | 0 16.28 | ~AAAA |
| ATOM | 100 | | GLY | 129 | | 30.543 | | | | 0 15.69 | AAAA |
| ATOM | 1009 | | MET | 130 | | 32.479 | | | | 0 16.10 0 15.00 | AAAA |
| MOTA | 1010 | CA CA | MET | 130 | | 31.879 | | | | 0 13.35 | AAAA AAAA |
| MOTA | 1011 | | MET | 130 | : | 32.969 | | 51.689 | 1.0 | 0 12.20 | AAAA |
| ATOM | 1012 | | MET | 130 | | 33.680 | | | 1.0 | 0 17.03 | AAAA |
| MOTA | 1013 1014 | | MET | 130 | | 34.863 | | | | 0 15.41 | AAAA |
| MOTA MOTA | 1019 | | MET MET | 130 130 | | 33.752 | | | | 0 46.82 | AAAA |
| ATOM | 1016 | _ | MET | 130 | | 31.296 31.785 | | | | 0 12.49 | AAAA |
| ATOM | 1017 | | HÌS | 131 | | 0.188 | | | | 0 19.54 0 16.24 | AAAA |
| MOTA | 1018 | CA | HIS | 131 | | 9.556 | | | | 0 13.80 | AAAA AAAA |
| MOTA | 1019 | | HIS | 131 | 2 | 8.772 | | 55.316 | 1.00 | 0 15.91 | AAAA |
| ATOM | 1020 | | HIS | 131 | | 7.606 | | | 1.00 | 13.08 | AAAA |
| ATOM | 1021 1022 | | HIS | 131 | | 6.712 | 30.063 | | | 12.46 | AAAA |
| MOTA MOTA | 1022 | | HIS | 131 131 | | 7.225 | 30.190 | | | 22.48 | AAAA |
| ATOM | 1024 | | HIS | 131 . | | 6.148 5.817 | 30.936 30.875 | | | 16.56 | AAAA |
| ATOM | 1025 | c | HIS | 131 | | 8.673 | 27.663 | | | 23.56 13.69 | AAAA |
| ATOM | 1026 | 0 | HIS | 131 | | 8.125 | 26.658 | 53.470 | - | 7 13.09 | AAAA AAAA |
| MOTA | 1027 | N | HIS | 132 | | 8.523 | 28.115 | 51.830 | | 14.51 | AAAA |
| MOTA | 1028 | CA | HIS | 132 | 2 | 7.669 | 27.400 | 50.887 | | 20.19 | AAAA |
| ATOM | 1029 | CB | HIS | 132 | | 6.863 | 28.416 | 50.054 | | 17.26 | AAAA |
| ATOM ATOM | 1030 1031 | CG | HIS HIS | 132 132 | | 5.748 | 29.070 | 50.810 | | 16.85 | AAAA |
| ATOM | 1032 | | HIS | 132 | | 4.787 5. 4 97 | 28.542 | 51.604 | | 13.74 | AAAA |
| ATOM | 1033 | | HIS | 132 | | 4.429 | 30.424 30.700 | 50.756 51.486 | | 24.80 12.68 | AAAA |
| ATOM | 1034 | NE2 | HIS | 132 | | 3.980 | 29.576 | 52.010 | | 28.65 | AAAA AAAA |
| ATOM | 1035 | С | HIS | 132 | | 3.372 | 26.412 | 49.946 | | 16.89 | AAAA |
| ATOM | 1036 |) | HIS | 132 | 27 | 7.731 | 25.487 | 49.460 | | 14.58 | AAAA |
| ATOM | 1037 | .7 | ALA | 133 | | 669 | 26.580 | 49.689 | | 16.79 | AAAA |
| ATOM ATOM | 1038 1039 | CA CB | ALA ALA | 133 133 | | 338 | 25.680 | 48.740 | | 13.76 | AAAA |
| ATOM | 1040 | C | ALA | 133 | | 1.738).418 | 26.194 | 48.412 | | 14.95 | AAAA |
| ATOM | 1041 | õ | ALA | 133 | | 1.557 | 24.219 23.939 | 49.179 50.355 | | 18.80 16.86 | AAAA |
| ATOM | 1042 | 71 | PHE | 134 | | .306 | 23.306 | 48.209 | | 13.76 | AAAA AAAA |
| MOTA | 1043 | CA | PHE | 134 | | .378 | 21.868 | 48.451 | | 19.77 | · AAAA |
| MOTA | 1044 | CB | PHE | 134 | | .311 | 21.132 | 47.620 | | 15.59 | AAAA |
| ATOM | 1045 | | PHE | 134 | | .917 | 21.525 | 47.975 | | 17.22 | AAAA |
| MOTA | 1046 | CD1 | | 134 | | .135 | 22.259 | 47.091 | 1.00 | 17.88 | AAAA |
| MOTA | 1047 | CD2 | | 134 | | .392 | 21.187 | 49.222 | | 21.68 | AAAA |
| ATOM ATOM | 1048 1049 | CE1 CE2 | | 134 134 | | .836 | 22.653 | 47.445 | | 23.07 | AAAA |
| ATOM | 1050 | | PHE PHE | 134 | | .099 .323 | 21.578 22.308 | 49.585 | | 17.64 | AAAA |
| ATOM | 1051 | | PHE | 134 | | .763 | 21.354 | 48.696 48.098 | | 19.71 14.76 | AAAA |
| MOTA | 1052 | | PHE | 134 | | .547 | 22.049 | 47.442 | | 18.05 | аааа Аааа |
| MOTA | 1053 | | LYS | 135 | | .060 | 20.124 | 48.515 | | 16.37 | AAAA |
| MOTA | 1054 | | LYS | 135 | | .369 | 19.551 | 48.269 | | 16.24 | AAAA |
| MOTA | 1055 | | LYS | 135 | | .360 | 18.070 | 48.699 | 1.00 | 21.29 | AAAA |
| MOTA | 1056 | CG I | LYS | 135 | 34 | . 640 | 17.300 | 48.400 | 1.00 | 30.43 | AAAA |
| | | | | | | | | | | | |

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Figure 16-17

| | 4055 | | | | | | | |
|------|------|--------|---------|----------------|--------|--------|------------|-------------|
| ATOM | 1057 | CD | LYS 13! | 34.597 | 15.867 | 48.977 | 1.00 30.26 | AAAA |
| ATOM | 1058 | CE 1 | LYS 13! | 34.862 | 15.805 | 50.486 | 1.00 35.01 | |
| | | | | | | | 1.00 33.01 | AAAA |
| ATOM | 1059 | NZ I | LYS 135 | 36.304 | 16.023 | 50.895 | 1.00 20.61 | AAAA |
| ATOM | 1060 | CI | LYS 135 | 33.854 | 19.687 | 46.836 | 1.00 16.60 | AAAA |
| ATOM | 1061 | | LYS 135 | | 20.020 | 46.584 | | |
| | | | | | | | 1.00 17.24 | AAAA |
| ATOM | 1062 | N S | SER 136 | 32.944 | 19.483 | 45.893 | 1.00 18.01 | AAAA |
| MOTA | 1063 | CA S | SER 136 | 33.301 | 19.528 | 44.490 | 1.00 15.26 | AAAA |
| | | | | | | | 1.00 13.20 | |
| ATOM | 1064 | CB S | SER 136 | 33.339 | 18.094 | 43.940 | 1.00 18.07 | AAAA |
| ATOM | 1065 | OG S | SER 136 | 34.135 | 17.261 | 44.762 | 1.00 22.22 | AAAA |
| | 1066 | | SER 136 | | 20.355 | | | |
| ATOM | | | | | | 43.658 | 1.00 15.40 | AAAA |
| ATOM | 1067 | 0 5 | SER 136 | 32.162 | 20.071 | 42.475 | 1.00 18.77 | AAAA |
| ATOM | 1068 | N P | ARG 137 | 31.754 | 21.401 | 44.237 | 1.00 19.71 | AAAA |
| | | | | | | | | |
| MOTA | 1069 | CA A | ARG 137 | 30.805 | 22.216 | 43.482 | 1.00 17.29 | AAAA |
| MOTA | 1070 | CB A | ARG 137 | 29.481 | 21.448 | 43.366 | 1.00 24.19 | AAAA |
| ATOM | 1071 | | RG 137 | | 22.273 | 42.937 | 1.00 32.56 | |
| | | | | | | | | AAAA |
| ATOM | 1072 | CD A | ARG 137 | 27.026 | 21.424 | 42.980 | 1.00 47.98 | AAAA |
| MOTA | 1073 | NE A | RG 137 | 26.951 | 20.493 | 41.862 | 1.00 50.95 | AAAA |
| | | | | | | | | |
| ATOM | 1074 | | ARG 137 | | 20.781 | 40.691 | 1.00 50.38 | AAAA |
| ATOM | 1075 | NH1 A | RG 137 | .25.854 | 21.976 | 40.485 | 1.00 45.26 | AAAA |
| ATOM | 1076 | NH2 A | | | 19.876 | 39.722 | 1.00 55.31 | AAAA |
| | | | | | | | | |
| MOTA | 1077 | C A | RG 137 | 30.537 | 23.595 | 44.095 | 1.00 16.14 | AAAA |
| MOTA | 1078 | O A | RG 137 | 30.439 | 23.711 | 45.308 | 1.00 16.88 | AAAA |
| ATOM | 1079 | | LA 138 | | 24.621 | | | |
| | | | | | | 43.252 | 1.00 18.07 | AAAA |
| ATOM | 1080 | CA A | LA 138 | 30.117 | 25.976 | 43.735 | 1.00 21.48 | AAAA |
| MOTA | 1081 | CB A | LA 138 | 30.460 | 27.024 | 42.631 | 1.00 16.55 | AAAA |
| | | | | | | | | |
| MOTA | 1082 | | LA 138 | 28.642 | 26.090 | 44.135 | 1.00 21.04 | AAAA |
| ATOM | 1083 | O A | LA 138 | 27.798 | 25.339 | 43.641 | 1.00 18.97 | AAAA |
| ATOM | 1084 | N A | SN 139 | 28.321 | 27.019 | 45.029 | 1.00 13.83 | AAAA |
| | | | | | | | | |
| MOTA | 1085 | | SN 139 | 26.952 | 27.158 | 45.468 | 1.00 12.92 | AAAA |
| ATOM | 1086 | CB A | SN 139 | 26.566 | 25.899 | 46.274 | 1.00 13.14 | AAAA |
| MOTA | 1087 | CG A | SN 139 | 25.162 | 25.961 | 46.832 | 1.00 20.34 | AAAA |
| | | | | | | | | |
| ATOM | 1088 | OD1 A | | 24.186 | 26.068 | 46.086 | 1.00 19.76 | AAAA |
| ATOM | 1089 | ND2 A | SN 139 | 25.048 | 25.881 | 48.157 | 1.00 16.36 | AAAA |
| ATOM | 1090 | | SN 139 | 26.756 | 28.409 | 46.315 | 1.00 20.92 | AAAA |
| | | | | | | | | |
| MOTA | 1091 | O A | SN 139 | 27 .603 | 28.738 | 47.148 | 1.00 16.81 | AAAA |
| ATOM | 1092 | N G | LY 140 | 25.644 | 29.105 | 46.086 | 1.00 19.30 | AAAA |
| | 1093 | | LY 140 | 25.330 | 30.295 | 46.864 | 1.00 21.34 | AAAA |
| ATOM | | | | | | | | |
| ATOM | 1094 | C G1 | LY 140 | 26.393 | 31.378 | 46.888 | 1.00 20.19 | AAAA |
| ATOM | 1095 | O G1 | LY 140 | 26.653 | 31.968 | 47.943 | 1.00 18.77 | AAAA |
| | 1096 | | HE 141 | 26.996 | 31.649 | 45.733 | 1.00 15.52 | |
| MOTA | | | | | | | | AAAA |
| ATOM | 1097 | CA PI | HE 141 | 28.034 | 32.675 | 45.600 | 1.00 20.71 | AAAA |
| ATOM | 1098 | CB PI | HE 141 | 27.711 | 33.952 | 46.388 | 1.00 20.03 | AAAA |
| | 1099 | | HE 141 | 26.355 | 34.544 | 46.127 | 1.00 28.32 | AAAA |
| MOTA | | | | | | | | |
| ATOM | 1100 | CD1 Pi | HE 141 | 25.855 | 35.526 | 46.997 | 1.00 24.25 | AAAA |
| ATOM | 1101 | CD2 PI | HE 141 | 25.589 | 34.170 | 45.029 | 1.00 30.11 | AAAA |
| | 1102 | CE1 Pi | | 24.628 | 36.116 | 46.775 | 1.00 25.94 | AAAA |
| ATOM | | | | | | | | |
| ATOM | 1103 | CE2 PF | HE 141 | 24.346 | 34.766 | 44.801 | 1.00 21.6: | AAAA |
| ATOM | 1104 | CZ PH | IE 141 | 23.870 | 35.741 | 45.677 | 1.00 24.4 | AAAA |
| ATOM | 1105 | C PH | | 29.357 | 32.188 | 46.158 | 1.00 14.45 | AAAA |
| | | | | | | | | |
| MOTA | 1106 | O PH | E 141 | 30.336 | 32.914 | 46.111 | 1.00 16.39 | AAAA |
| ATOM | 1107 | N CY | 'S 142 | 29.389 | 30.982 | 46.716 | 1.00 16.77 | AAAA |
| | | | | 30.629 | 30.466 | 47.285 | 1.00 17.71 | AAAA |
| MOTA | 1108 | CA CY | | | | | | |
| ATOM | 1109 | CB CY | 'S 142 | 30.347 | 29.845 | 48.659 | 1.00 13.95 | AAAA |
| ATOM | 1110 | SG CY | S 142 | 29.606 | 30.985 | 49.846 | 1.00 16.63 | AAAA |
| | | | | | | | | |
| MOTA | 1111 | C CX | | 31.313 | 29.421 | 46.401 | 1.00 18.09 | AAAA |
| ATOM | 1112 | O CY | S 142 | 30.647 | 28.527 | 45.856 | 1.00 16.60 | AAAA |
| | 1113 | N TY | | 32.639 | 29.539 | 46.272 | 1.00 12.50 | AAAA |
| MOTA | | | | | | | | |
| ATOM | 1114 | CA TY | | 33.429 | 28.603 | 45.478 | 1.00 15.32 | AAAA |
| MOTA | 1115 | CB TY | R 143 | 34.333 | 29.322 | 44.473 | 1.00 13.07 | AAAA |
| | 1116 | CG TY | | 33.614 | 30.338 | 43.612 | 1.00 15.80 | AAAA |
| MOTA | | | | | | | | |
| ATOM | 1117 | CD1 TY | | 33.396 | 31.636 | 44.071 | 1.00 15.48 | AAAA |
| MOTA | 1118 | CE1 TY | R 143 | 32.740 | 32.589 | 43.270 | 1.00 11.99 | AAAA |
| | | CD2 TY | | 33.157 | 29.999 | 42.336 | 1.00 14.60 | AAAA |
| ATOM | 1119 | | | | | | | |
| MOTA | 1120 | CE2 TY | | 32.501 | 30.935 | 41.532 | 1.00 10.74 | AAAA |
| ATOM | 1121 | CZ TY | R 143 | 32.301 | 32.229 | 42.008 | 1.00 20.89 | AAAA |
| | | | | 31.698 | 33.177 | 41.208 | 1.00 18.87 | AAAA |
| ATOM | 1122 | OH TY | v ra2 | 31.030 | 22.1/ | 31.200 | 1.00 10.07 | |
| | | • | | | | | | • |

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| ATOM | 1 112 | 23 (| TYI | R 143 | 34.33 | 10 27.72 | 3 46.358 | 3 1.00 17.35 | |
|--------|-------|------|------------|-------------|--------|----------|----------|--------------|--------|
| ATOM | 1 112 | 24 (| TY! | R 143 | 34.58 | | | | |
| ATOM | 1 112 | 25 1 | J ILI | E 144 | 34.76 | | | | |
| MOTA | 112 | 26 C | A ILE | 3 144 | 35.59 | | | | |
| ATOM | 112 | :7 c | B ILE | 144 | 37.01 | | | | |
| ATOM | 112 | 8 C | G2 ILE | | 37.86 | | | | AAAA |
| ATOM | 112 | | G1 ILE | | 37.61 | | | | AAAA |
| MOTA | 113 | | D1 ILE | | 39.05 | | | | AAAA |
| ATOM | 113 | | | _ | 34.95 | | | | AAAA |
| ATOM | | | | | 34.60 | _ | | | AAAA |
| ATOM | | | | | 34.79 | | | | , AAAA |
| ATOM | | | | | 34.17 | | | | AAAA |
| ATOM | | - | | | 33.40 | | | | AAAA |
| ATOM | | _ | | | 32.42 | | | | AAAA |
| MOTA | 113 | | D1 ASN | | | | | | AAAA |
| ATOM | 113 | | D2 ASN | | 32.80 | | | | AAAA |
| ATOM | 113 | | ASN ASN | | | _ | | | AAAA |
| ATOM | 114 | _ | ASN | | 35.26 | | | | AAAA |
| ATOM | 114: | | | | 35.81 | | | | AAAA |
| ATOM | 114 | | | | 35.59 | | | | AAAA |
| ATOM | 1143 | | | 146 | 36.68 | | | | AAAA |
| ATOM | 1144 | | | 146 | 37.16: | | | 1.00 15.81 | AAAA |
| | | | | 146 | 36.10 | | | 1.00 15.25 | AAAA |
| ATOM | 1145 | | Ol ASN | 146 | | | | 1.00 13.57 | AAAA |
| MOTA | 1146 | | 2 ASN | 146 | 35.156 | | 53.996 | 1.00 10.85 | AAAA |
| ATOM | 1147 | | ASN | 146 | 36.306 | 27.400 | | 1.00 13.04 | AAAA |
| MOTA | 1148 | | ASN | 146 | 37.160 | | | 1.00 14.76 | AAAA |
| MOTA | 1149 | | PRO | 147 | 35.025 | | 56.016 | 1.00 14.28 | AAAA |
| ATOM | 1150 | | | 147 | 33.817 | | | 1.00 7.62 | AAAA |
| ATOM | 1151 | | | 147 | 34.750 | | 57.307 | 1.00 13.51 | AAAA |
| ATOM | 1152 | | | 147 | 33.251 | | | 1.00 14.44 | AAAA |
| MOTA | 1153 | | | 147 | 33.056 | | 56.827 | 1.00 12.32 | AAAA |
| MOTA | 1154 | | PRO | 147 | 35.118 | | 57.278 | 1.00 18.86 | AAAA |
| ATOM | 1155 | | PRO | 147 | 35.678 | 24.796 | 58.251 | 1.00 16.24 | AAAA |
| ATOM | 1156 | | ALA | 148 | 34.818 | | | 1.00 15.01 | AAAA |
| MOŢA | 1157 | CA | ALA | 148 | 35.122 | 23.200 | | 1.00 15.58 | AAAA |
| MOTA | 1158 | CB | ALA | 148 | 34.402 | | 54.882 | 1.00 12.93 | AAAA |
| ATOM | 1159 | С | ALA | 148 | 36.624 | | 55.984 | 1.00 14.94 | AAAA |
| MOTA | 1160 | 0 | ALA | 148 | 37.138 | 21.999 | 56.560 | 1.00 14.69 | AAAA |
| MOTA | 1161 | N | VAL | 149 | 37.328 | 23.817 | 55.263 | 1.00 12.49 | AAAA |
| ATOM | 1162 | CA | VAL | 149 | 38.778 | 23.708 | 55.163 | 1.00 15.31 | AAAA |
| ATOM | 1163 | CB | VAL | 149 | 39.364 | 24.797 | 54.243 | 1.00 14.77 | AAAA |
| MOTA | 1164 | | L VAL | 149 | 40.899 | 24.870 | 54.369 | 1.00 14.68 | AAAA |
| MOTA | 1165 | CG2 | VAL | 149 | 38.981 | 24.501 | 52.808 | 1.00 12.50 | AAAA |
| ATOM | 1166 | С | VAL | 149 | 39.323 | 23.887 | 56.572 | 1.00 20.14 | AAAA |
| ATOM | 1167 | 0 | VAL | 149 | 40.172 | 23.109 | 57.028 | 1.00 17.32 | |
| ATOM | 1168 | N | GLY | 50 | 38.815 | 24.899 | 57.271 | 1.00 15.45 | AAAA |
| ATOM | 1169 | CA | GLY | _50 | 39.284 | 25.168 | 58.622 | 1.00 20.96 | AAAA |
| ATOM | 1170 | С | GLY | - 50 | 39.030 | 24.053 | 59.621 | 1.00 24.16 | AAAA |
| MOTA | 1171 | 0 | GLY | 150 | 39.888 | 23.738 | 60.458 | 1.00 19.50 | AAAA |
| ATOM | 1172 | N | ILE | 151 | 37.842 | 23.465 | 59.557 | 1.00 16.67 | AAAA |
| ATOM | 1173 | CA | ILE | 151 | 37.490 | | 60.461 | 1.00 19.56 | AAAA |
| ATOM | 1174 | CB | ILE | 151 | 35.992 | 22.052 | 60.348 | | AAAA |
| ATOM | 1175 | CG2 | ILE | 151 | 35.667 | 20.709 | 61.036 | 1.00 16.46 | AAAA |
| ATOM | 1176 | | ILE | 151 | 35.180 | 23.209 | | 1.00 17.93 | AAAA |
| MOTA | 1177 | | ILE | 151 | 33.686 | 23.123 | 60.959 | 1.00 12.31 | AAAA |
| ATOM | 1178 | c | ILE | 151 | 38.352 | | 60.672 | 1.00 18.71 | AAAA |
| ATOM | 1179 | ō | ILE | 151 | 38.796 | 21.148 | 60.164 | 1.00 22.66 | AAAA |
| ATOM | 1180 | N | GLU | 152 | 38.599 | 20.472 | 61.087 | 1.00 20.08 | AAAA |
| | 1181 | CA | GLU | 152 | | 20.861 | 58.888 | 1.00 19.71 | AAAA |
| ATOM | 1182 | CB | GLU | 152 | 39.434 | 19.718 | 58.533 | 1.00 13.85 | AAAA |
| ATOM | 1182 | | | | 39.362 | 19.437 | 57.033 | 1.00 20.21 | AAAA |
| | 1184 | CG . | GLU | 152 | 38.033 | 18.833 | 56.624 | 1.00 22.16 | AAAA |
| ATOM | | CD | GLU | 152 | 37.838 | 17.430 | 57.166 | 1.00 26.94 | AAAA |
| ATOM | 1185 | 0E1 | | 152 | 36.720 | 16.906 | 57.035 | 1.00 25.03 | AAAA |
| ATCM . | 1186 | OE2 | | 152 | 38.800 | 16.846 | 57.708 | 1.00 24.95 | AAAA |
| ATOM | 1187 | | GLU | 152 | 40.865 | 20.010 | | 1.00 16.85 | AAAA |
| ATCM | 1188 | O | GLU ' | 152 | 41.629 | 19.110 | | 1.00 19.25 | AAAA |
| | | | | | | | • | * | |

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| | | | | | | • | | | | | |
|--------------|--------------|--------|------------|------------|---|------------------|------------------|------------------|------|----------------|--------------|
| ATOM | 1189 | N | .TYR | 153 | | 41.228 | 21.290 | 58.931 | 1.00 | 14.74 | AAAA |
| MOTA | 1190 | CA | TYR | 153 | | 42.574 | 21.672 | 59.350 | | 17.71 | AAAA |
| MOTA | 1191 | CB | TYR | 153 | | 42.757 | 23.193 | 59.179 | | 13.26 | AAAA |
| ATOM | 1192 | CG | TYR | 153 | | 44.059 | 23.727 | 59.729 | 1.00 | 16.36 | AAAA |
| MOTA | 1193 | CD | 1 TYR | 153 | | 45.234 | 23.726 | 58.967 | | 18.41 | AAAA |
| MOTA | 1194 | CE | 1 TYR | 153 | | 46.438 | 24.219 | 59.511 | 1.00 | 21.03 | AAAA |
| ATOM | 1195 | CD | 2 TYR | 153 | | 44.115 | 24.220 | 61.028 | 1.00 | 21.16 | AAAA |
| ATOM | 1196 | CE | 2 TYR | 153 | | 45.288 | 24.705 | 61.570 | 1.00 | 19.76 | AAAA |
| ATOM | 1197 | CZ | TYR | 153 | | 46.440 | 24.711 | 60.824 | 1.00 | 25.97 | AAAA |
| ATOM | 1198 | OH | TYR | 153 | | 47.571 | 25.235 | 61.410 | 1.00 | 23.15 | AAAA |
| MOTA | 1199 | С | TYR | 153 | - | 42.712 | 21.274 | 60.828 | 1.00 | 20.00 | AAAA |
| ATOM | 1200 | 0 | TYR | 153 | | 43.722 | 20.698 | 61.247 | 1.00 | 19.61 | AAAA |
| ATOM | 1201 | N | LEU | 154 | | 41.683 | 21.569 | 61.616 | 1.00 | 17.78 | AAAA |
| MOTA | 1202 | CA | LEU | 154 | | 41.698 | 21.239 | 63.042 | 1.00 | 17.26 | AAAA |
| MOTA | 1203 | CB | LEU | 154 | | 40.511 | 21.913 | 63.744 | 1.00 | 20.44 | AAAA |
| MOTA | 1204 | CG | LEU | 154 | | 40.636 | 23.434 | 63.942 | 1.00 | 19.57 | AAAA |
| MOTA | 1205 | | l LEU | 154 | | 39.277 | 24.046 | 64.309 | 1.00 | 22.48 | AAAA |
| MOTA | 1206 | | 5 FER | 154 | | 41.692 | 23.709 | 65.044 | 1.00 | 20.84 | AAAA |
| MOTA | 1207 | С | LEU | 154 | | 41.669 | 19.715 | 63.262 | 1.00 | 19.69 | AAAA |
| ATOM | 1208 | 0 | LEU | 154 | | 42.357 | 19.191 | 64.149 | 1.00 | 22.91 | AAAA |
| ATOM | 1209 | N | ARG | 155 | | 40.878 | 18.996 | 62.469 | | 20.88 | . AAAA |
| MOTA | 1210 | CA | ARG | 155 | | 40.840 | 17.539 | 62.622 | | 22.64 | AAAA |
| MOTA | 1211 | CB | ARG | 155 | | 39.829 | 16.905 | 61.652 | | 25.69 | AAAA |
| MOTA | 1212 | CG | ARG | 155 | | 38.384 | 17.394 | 61.893 | | 27.64 | AAAA |
| MOTA | 1213 | CD | ARG | 155 | | 37.382 | 16.834 | 60.892 | | 25.67 | AAAA |
| ATOM | 1214 | NE | ARG | 155 | | 36.931 | 15.497 | 61.246 | | 30.88 | AAAA |
| MOTA | 1215 | CZ | ARG | 155 | | 36.135 | 14.753 | 60.488 | | 36.28 | AAAA |
| ATOM | 1216 | | ARG | 155 | • | 35.705 | 15.218 | 59.318 | | 26.96 | AAAA |
| ATOM | 1217 1218 | NH2 | | 155 | | 35.737 | 13.562 16.966 | 60.923 | | 27.33 | AAAA |
| MOTA | 1219 | С 0 | ARG ARG | 155 155 | | 42.235 42.674 | 16.988 | 62.390 63.119 | | 28.00 | AAAA |
| MOTA MOTA | 1220 | И | LYS | 156 | | 42.949 | 17.486 | 61.395 | | 28.05 23.53 | AAAA AAAA |
| ATOM | 1221 | CA | LYS | 156 | | 44.290 | 16.977 | 61.128 | | 26.79 | AAAA |
| ATOM | 1222 | CB | LYS | 156 | | 44.854 | 17.558 | 59.824 | | 26.01 | AAAA |
| ATOM | 1223 | CG | LYS | 156 | | 46.213 | 16.955 | 59.444 | | 29.70 | AAAA |
| ATOM | 1224 | CD | LYS | 156 | | 46.632 | 17.308 | 58.035 | | 28.77 | AAAA |
| ATOM | 1225 | CE | LYS | 156 | | 45.685 | 16.692 | 57.005 | | 39.79 | AAAA |
| ATOM | 1226 | NZ | LYS | 156 | | 45.671 | 15.192 | 57.058 | | 36.33 | AAAA |
| ATOM | 1227 | C | LYS | 156 | | 45.233 | 17.260 | 62.299 | 1.00 | 26.40 | AAAA |
| ATOM | 1228 | 0 | LYS | 156 | | 46.188 | 16.511 | 62.529 | 1.00 | 26.19 | AAAA |
| MOTA | 1229 | N | LYS | 157 | • | 44.960 | 18.337 | 63.032 | 1.00 | 22.50 | AAAA |
| MOTA | 1230 | CA | LYS | 157 | | 45.757 | 18.709 | 64.204 | | 21.12 | AAAA |
| ATOM | 1231 | CB | LYS | 157 | | 45.535 | 20.181 | 64.591 | | 28.95 | AAAA |
| ATOM | 1232 | CG | LYS | 157 | | 46.160 | 21.215 | 63.652 | | 25.94 | AAAA |
| ATOM | 1233 | CD | LYS | 157 | | 47.669 | 21.067 | 63.575 | | 35.16 | AAAA |
| MOTA | 1234 | CE | LYS | 157 | | 48.281 | 22.099 | 62.627 | | 39.24 | AAAA |
| ATOM | 1235 | NZ | LYS | 157 | | 49.742 | 21.869 | 62.406 | | 40.01 | AAAA |
| MOTA | 1236 | C | LYS | 157 | | 45.421 | 17.825 | 65.411 | | 22.98 | AAAA |
| ATCM | 1237 1238 | O N | LYS GLY | 157 158 | | 46.085 44.392 | 17.903 16.995 | 66.444 65.284 | | 27.77 26.49 | AAAA AAAA |
| ATCM | 1239 | CA | GLY | 158 | | 44.392 | | 66.376 | | 24.82 | AAAA |
| ATOM ATOM | 1240 | C | GLY | 158 | | 42.771 | 16.459 | 67.161 | | 33.13 | AAAA |
| ATOM | 1241 | ō | GLY | 158 | | 42.421 | 15.775 | 68.128 | | 27.21 | AAAA |
| ATOM | 1242 | N | PHE | 159 | | 42.085 | 17.529 | 66.781 | | 27.47 | AAAA |
| ATOM | 1243 | CA | PHE | 159 | | 40.866 | 17.861 | 67.502 | | 24.15 | AAAA |
| ATOM | 1244 | СВ | PHE | 159 | | 40.410 | 19.285 | 67.186 | | 27.53 | AAAA |
| ATOM | 1245 | CG | PHE | 159 | | 41.264 | 20.343 | 67.827 | | 27.26 | AAAA |
| ATOM | 1246 | | PHE | 159 | | 42.439 | 20.785 | 67.220 | | 28.12 | AAAA |
| ATOM | 1247 | | PHE | 159 | | 40.926 | 20.842 | 69.076 | | 21.10 | AAAA |
| ATCM | 1248 | | PHE | 159 | | 43.264 | 21.714 | 67.866 | | 26.24 | AAAA |
| ATOM | 1249 | | PHE | 159 | | 41.738 | 21.768 | 69.736 | | 26.07 | AAAA |
| ATOM | 1250 | CZ | PHE | 159 | | 42.907 | 22.205 | 69.135 | 1.00 | 23.91 | AAAA |
| ATOM | 1251 | C | PHE | 159 | | 39.792 | 16.854 | 67.120 | | 28.02 | AAAA |
| ATCM | 1252 | 0 | PHE | 159 | | 39.639 | 16.533 | 65.947 | 1.00 | 21.14 | AAAA |
| ATCM | 1253 | N | LYS | 160 | | 39.056 | 16.361 | 68.110 | | 24.79 | AAAA |
| ATOM | 1254 | CA | LYS | 160 | | 38.011 | 15.366 | 67.881 | 1.00 | 24.26 | AAAA |

| • | | | | | | |
|--------------------------------|--------------------------|------------------|--------------------|------------------|--------------------------|----------------|
| | CB LYS 160 | 38.360 | 0 14.098 | 68.668 | 1.00 22.86 | |
| | CG LYS 160 | 39.629 | 5 13.424 | | 1.00 43.16 | AAAA |
| | CD LYS 160 CE LYS 160 | 40.222 | | 69.141 | 1.00 54.05 | AAAA AAAA |
| | | 39.236 | | | 1.00 62.87 | AAAA |
| | NZ LYS 160 C LYS 160 | 38.154 | | | 1.00 68.11 | AAAA |
| | 0 LYS 160 | 36.599 | | | 1.00 21.12 | AAAA |
| | N ARG 161 | 35.632 36.476 | | 68.051 | 1.00 22.43 | AAAA |
| | CA ARG 161 | 35.164 | | 68.733 | 1.00 19.68 | AAAA |
| | CB ARG 161 | 34.865 | | 69.073 | 1.00 20.84 | AAAA |
| ATOM 1265 C | CG ARG 161 | 34.715 | 16.031 | 70.572 71.080 | 1.00 26.02 | AAAA |
| | D ARG 161 | 34.213 | | 72.523 | 1.00 28.47 | AAAA |
| | VE ARG 161 | 35.098 | | 73.445 | 1.00 30.38 1.00 32.99 | AAAA |
| | Z ARG 161 | 36.272 | | 73.883 | 1.00 32.99 | AAAA |
| | H1 ARG 161 | 36.724 | 15.094 | 73.489 | 1.00 31.49 | AAAA |
| | H2 ARG 161 | 37.003 | 17.014 | 74.712 | 1.00 38.54 | AAAA |
| ATOM 1271 C ATOM 1272 O | | 35.171 | 19.060 | 68.680 | 1.00 18.98 | AAAA - AAAA |
| | | 35.552 | 19.932 | 69.460 | 1.00 23.57 | AAAA |
| ATOM 1273 N ATOM 1274 C | | 34.743 | 19.332 | 67.458 | 1.00 19.82 | AAAA |
| ATOM 1275 CI | | 34.744 | 20.700 | 66.947 | 1.00 17.81 | AAAA |
| | B ILE 162 G2 ILE 162 | 35.522 | 20.717 | 65.626 | 1.00 18.33 | AAAA |
| | G1 ILE 162 | 35.542 36.937 | 22.110 | 65.042 | 1.00 13.65 | AAAA |
| | D1 ILE 162 | 37.722 | 20.200 | 65.895 | 1.00 18.15 | AAAA |
| ATOM 1279 C | ILE 162 | 33.316 | 19.852 21.184 | 64.670 | 1.00 22.52 | AAAA |
| ATOM 1280 O | ILE 162 | 32.520 | 20.492 | 66.724 | 1.00 14.71 | AAAA |
| ATOM 1281 N | LEU 163 | 32.996 | 22.374 | 66.126 67.217 | 1.00 17.99 | AAAA |
| ATOM 1282 CA | | 31.653 | 22.902 | | 1.00 16.93 1.00 20.73 | AAAA |
| ATOM 1283 CB | | 31.115 | 23.376 | | 1.00 18.45 | AAAA |
| ATOM 1284 CG | | 29.846 | 24.236 | 68.463 . | 1.00 19.99 | AAAA AAAA |
| | 1 LEU 163 | 28.657 | 23.408 | 67.975 | 1.00 15.66 | AAAA |
| ATOM 1287 C | 2 LEU 163 LEU 163 | 29.609 | 24.751 | 69.870 | 1.00 18.74 | AAAA |
| ATOM 1288 0 | LEU 163 LEU 163 | 31.705 | 24.071 | 66.106 | 1.00 18.40 | AAAA |
| ATOM 1289 N | TYR 164 | 32.607 30.752 | 24.889 | 66.188 | 1.00 18.65 | AAAA |
| ATOM 1290 CA | | 30.656 | 24.128 25.246 | | 1.00 16.97. | AAAA |
| ATOM 1291 CB | TYR 164 | 30.782 | 24.754 | 64.252 | 1.00 11.76 | AĄĄA |
| ATOM 1292 CG | TYR 164 | 30.593 | | 62.816 61.797 | 1.00 14.07 1.00 14.51 | AAAA |
| ATOM 1293 CD1 | | 31.573 | | | 1.00 14.51 | AAAA |
| | 1 TYR 164 | 31.353 | | | 1.00 26.21 | AAAA |
| ATOM 1295 CD2 ATOM 1296 CE2 | | 29.415 | | | 1.00 21.45 | AAAA AAAA |
| | | 29.193 | | | 1.00 21.89 | AAAA |
| ATOM 1297 CZ ATOM 1298 OH | TYR 164 | 30.148 | 27.839 | | 1.00 16.35 | AAAA |
| ATOM 1299 C | TYR 164 TYR 164 | 29.857 | 28.764 | 58.913 1 | 1.00 27.44 | AAAA |
| ATOM 1300 O | TYR 164 TYR 164 | | | 64.463 1 | .00 15.67 | AAAA |
| ATOM 1301 N | ILE 165 | | | | .00 16.07 | AAAA |
| ATOM 1302 CA | ILE 165 | | | | .00 14.52 | AAAA |
| ATOM 1303 CB | ILE 165 | 27.959 | | | .00 18.37 | AAAA |
| ATOM 1304 CG2 | ILE 165 | | | | .00 13.31 | AAAA |
| | ILE 165 | | | | .00 13.06 | AAAA |
| | ILE 165 | 28.493 | | | .00 17.28 .00 15.02 | AAAA |
| ATOM 1307 C | ILE 165 | 27.853 | | | .00 20.75 | AAAA AAAA |
| ATOM 1308 0 | ILE 165 | 28.759 | | | .00 16.67 | AAAA |
| | ASP 166 | | 28.901 6 | 3.084 1 | .00 15.37 | AAAA |
| | ASP 166 ASP 166 | | 29.779 6 | 1.942 1 | .00 15.63 | AAAA |
| | | | | 0.698 1 | .00 12.31 | AAAA |
| ATOM 1313 OD1 | | | | | .00 16.37 | AAAA |
| ATCM 1314 OD2 | ASP 166 | | | | .00 13.41 | AAAA |
| | ASP 166 | | 9.428 5 0.740 6 | 8.551 1. | .00 16.06 | AAAA |
| | ASP 166 | | - | | .00 15.54 | AAAA |
| | LEU 167 | | | | 00 12.60 | AAAA |
| ATOM 1318 CA 1 | LEU 167 | | | | 00 14.02 | AAAA |
| ATOM 1319 ÇB 1 | LEU 167 | | | | 00 12.05 00 14.61 | AAAA |
| ATCM 1320 CG I | LEU 167 | | 3.239 6 | | 00 14.81 | алад Алад |
| • • | | | | L. | 00 17.20 | AAAA |
| | | | | | | |

| ATOM | 1321 | CD1 | LEU | 167 | 25.635 | 34.271 | 66.169 | 1.00 28.82 | · AAAA |
|------|------|-----|-----|-------|--------|--------|----------------|------------|--------|
| ATOM | 1322 | CD2 | LEU | 167 | 24.148 | 32.372 | 65.513 | 1.00 18.59 | AAAA |
| | 1323 | c | LEU | | 24.122 | 33.776 | 61.449 | 1.00 12.62 | AAAA |
| ATOM | | Ö | | 167 | 23.288 | 34.678 | 61.570 | 1.00 15.00 | AAAA |
| MOTA | 1324 | | LEU | | | | | | |
| ATOM | 1325 | N | ASP | 168 | 24.667 | 33.431 | 60.288 | 1.00 14.35 | AAAA |
| ATOM | 1326 | CA | ASP | 168 | 24.277 | 34.056 | 59.022 | 1.00 19.50 | AAAA |
| MOTA | 1327 | CB | ASP | 168 | 25.060 | 33.409 | 57.880 | 1.00 25.15 | AAAA |
| ATOM | 1328 | CG | ASP | 168 | 24.908 | 34.145 | 56.573 | 1.00 48.45 | AAAA |
| ATOM | 1329 | ODI | ASP | 168 | 25.477 | 35.247 | 56.454 | 1.00 64.45 | AAAA |
| | 1330 | | ASP | 168 | 24.215 | 33.633 | 55.668 | 1.00 44.71 | AAAA |
| MOTA | | | | | | 33.751 | 58.834 | 1.00 16:30 | AAAA |
| MOTA | 1331 | C | ASP | 168 | 22.787 | | | | |
| MOTA | 1332 | 0 | ASP | 168 | 22.327 | 32.696 | 59.252 | 1.00 17.72 | AAAA |
| ATOM | 1333 | N | ALA | 169 | 22.059 | 34.657 | 58.175 | 1.00 14.11 | AAAA . |
| MOTA | 1334 | CA | ALA | 169 | 20.618 | 34.503 | 57.934 | 1.00 19.61 | AAAA |
| ATOM | 1335 | CB | ALA | 169 | 20.006 | 35.856 | 57.470 | 1.00 13.56 | AAAA |
| MOTA | 1336 | С | ALA | 169 | 20.277 | 33.400 | 56.926 | 1.00 18.23 | AAAA |
| ATOM | 1337 | ō | ALA | 169 | 19.105 | 33.159 | 56.641 | 1.00 17.20 | AAAA |
| | | N. | HIS | 170 | 21.301 | 32.750 | 56.373 | 1.00 16.53 | AAAA |
| MOTA | 1338 | | | | 21.075 | 31.652 | 55.436 | 1.00 17.51 | AAAA |
| MOTA | 1339 | CA | HIS | 170 | | | | | |
| MOTA | 1340 | CB | HIS | 170 | 21.616 | 31.973 | 54.033 | 1.00 22.32 | AAAA |
| ATOM | 1341 | CG | HIS | 170 | 20.954 | 33.142 | 53.377 | 1.00 25.38 | AAAA |
| ATOM | 1342 | CD2 | HIS | 170 | 19.934 | 33.196 | 52.487 | 1.00 19.33 | AAAA |
| ATOM | 1343 | ND1 | HIS | 170 | 21.308 | 34.448 | 53.638 | 1.00 18.17 | AAAA |
| ATOM | 1344 | | HIS | 170 | 20.535 | 35.257 | 52.935 | 1.00 30.34 | AAAA |
| ATOM | 1345 | | HIS | 170 | 19.692 | 34.523 | 52.229 | 1.00 17.51 | AAAA |
| | 1346 | С | HIS | 170 | 21.781 | 30.413 | 55.967 | 1.00 16.72 | AAAA |
| ATOM | | | | 170 | 22.827 | 30.511 | 56.610 | 1.00 15.92 | AAAA |
| ATOM | 1347 | 0 | HIS | | | | 55.682 | 1.00 15.28 | ÁAAA |
| ATOM | 1348 | N | HIS | 171 | 21.209 | 29.245 | | | |
| MOTA | 1349 | CA | HIS | 171 | 21.751 | 27.961 | 56.123 | 1.00 12.53 | AAAA |
| MOTA | 1350 | CB | HIS | 171 | 20.702 | 26.878 | 55.814 | 1.00 14.09 | AAAA |
| MOTA | 1351 | CG | HIS | 171 | 21.180 | 25.468 | 55.980 | 1.00 17.27 | AAAA |
| ATOM | 1352 | CD2 | HIS | 171 | 21.249 | 24.447 | 55.090 | 1.00 12.48 | AAAA |
| ATOM | 1353 | | HIS | 171 | 21.622 | 24.956 | 57.181 | 1.00 26.73 | AAAA |
| ATOM | 1354 | _ | HIS | 171 - | 21.948 | 23.685 | 57.021 | 1.00 15.98 | AAAA |
| | 1355 | | HIS | 171 | 21.729 | 23.352 | 55.761 | 1.00 20.03 | AAAA |
| ATOM | | | HIS | 171 | 23.107 | 27.602 | 55.498 | 1.00 15.55 | AAAA |
| MOTA | 1356 | C | | | | 27.784 | 54.298 | 1.00 17.03 | AAAA |
| MOTA | 1357 | 0 | HIS | 171 | 23.318 | | | 1.00 14.33 | AAAA |
| MOTA | 1358 | N | CYS | 172 | 24.026 | 27.105 | 56.323 | | |
| MOTA | 1359 | CA | CYS | 172 | 25.350 | 26.675 | 55.866 | 1.00 13.65 | AAAA |
| MOTA | 1360 | CB | CYS | 172 | 26.330 | 26.631 | 57.054 | 1.00 12.99 | AAAA |
| ATOM | 1361 | SG | CYS | 172 | 25.680 | 25.826 | 58.551 | 1.00 17.17 | AAAA |
| ATOM | 1362 | С | CYS | 172 | 25.212 | 25.274 | 5 5.257 | 1.00 16.52 | AAAA |
| ATOM | 1363 | 0 | CYS | 172 | 25.750 | 24.297 | 55.783 | 1.00 14.95 | AAAA |
| ATOM | 1364 | N | ASP | 173 | 24.516 | 25.173 | 54.130 | 1.00 15.42 | AAAA |
| | 1365 | CA | ASP | 173 | 24.302 | 23.865 | 53.531 | 1.00 14.75 | AAAA |
| ATOM | | | | 173 | 23.339 | 23.956 | 52.332 | 1.00 17.73 | AAAA |
| ATOM | 1366 | CB | ASP | | | | 51.283 | 1.00 22.84 | AAAA |
| ATOM | 1367 | CG | ASP | 173 | 23.765 | 24.966 | | | AAAA |
| MOTA | 1368 | | ASP | 173 | 23.106 | 24.998 | 50.216 | 1.00 18.68 | |
| ATOM | 1369 | OD2 | ASP | 173 | 24.730 | 25.728 | 51.504 | 1.00 15.34 | AAAA |
| ATOM | 1370 | С | ASP | 173 | 25.590 | 23.145 | 53.149 | 1.00 16.39 | AAAA |
| ATOM | 1371 | 0 | ASP | 173 · | 25.684 | 21.922 | 53.279 | 1.00 16.48 | AAAA |
| ATOM | 1372 | N | GLY | 174 | 26.583 | 23.912 | 52.705 | 1.00 15.58 | AAAA |
| | 1373 | CA | GLY | 174 | 27.869 | 23.346 | 52.360 | 1.00 13.97 | AAAA |
| ATOM | | C | GLY | 174 | 28.508 | 22.723 | 53.595 | 1.00 18.44 | AAAA |
| ATOM | 1374 | | | | 28.970 | 21.586 | 53.540 | 1.00 15.48 | AAAA |
| ATOM | 1375 | 0 | GLY | 174 | | | | 1.00 16.84 | AAAA |
| ATOM | 1376 | N | VAL | 175 | 28.554 | 23.456 | 54.706 | | AAAA |
| MOTA | 1377 | CA | ΛYΓ | 175 | 29.136 | 22.923 | 55.946 | 1.00 16.54 | |
| ATOM | 1378 | CB | VAL | 175 | 29.201 | 24.031 | 57.037 | 1.00 15.88 | AAAA |
| ATOM | 1379 | CG1 | VAL | 175 | 29.927 | 23.507 | 58.3 07 | 1.00 15.35 | AAAA |
| ATOM | 1380 | CG2 | | 175 | 29.923 | 25.258 | 56.476 | 1.00 15.62 | AAAA |
| | 1381 | c | VAL | 175 | 28.318 | 21.720 | 56.467 | 1.00 19.21 | AAAA |
| ATOM | | ō | VAL | 175 | 28.876 | 20.735 | 56.961 | 1.00 17.75 | AAAA |
| ATOM | 1382 | | | 176 | 26.996 | 21.798 | 56.367 | 1.00 17.74 | AAAA |
| MOTA | 1383 | N | GLN | | | | 56.832 | 1.00 15.66 | AAAA |
| ATOM | 1384 | CA | GLN | 176 | 26.164 | 20.685 | | 1.00 16.64 | AAAA |
| ATOM | 1385 | CB | GLN | 176 | 24.678 | 20.973 | 56.595 | 1.00 10.04 | |
| ATOM | 1386 | CG | GLN | 176 | 23.789 | 19.788 | 56.952 | 1.00 17.00 | AAAA . |
| • | | | - | | | | - | | • |

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| MOTA | 1387 | ' CD | GLN | 176 | 22.325 | 20.106 | 56.884 | 1.00 21.52 | AAAA |
|---------------------------------------|---------|------|--------|--------------|--------|--------------------|---------|------------|---------|
| | 1388 | OF | 1 GLN | 176 | 21.850 | 21.016 | 57.567 | 1.00 21.72 | |
| MOTA | | | | | | | | | AAAA |
| MOTA | 1389 | NE | 2 GLN | 176 | 21.581 | 19.348 | 56.064 | 1.00 20.30 | AAAA |
| ATOM | 1390 |) С | GLN | 176 | 26.527 | 19.387 | 56.121 | 1.00 16.33 | AAAA |
| | | | | | | | | | |
| ATOM | 1391 | . 0 | GLN | 176 | 26.751 | 18.354 | 56.748 | 1.00 17.46 | AAAA |
| ATOM | 1392 | N | GLU | 177 | 26.581 | 19.443 | 54.799 | 1.00 22.24 | AAAA |
| | | | | | | | | | |
| ATOM | 1393 | CA | GLU | 177 | 26.909 | 18.251 | 54.021 | 1.00 19.67 | AAAA |
| MOTA | 1394 | CB | GLU | 177 | 26.857 | 18.587 | 52.533 | 1.00 15.55 | AAAA |
| | | | | | | | | | |
| MOTA | 1395 | CG | GLU | 1 7 7 | 27.131 | 17.388 | 51.623 | 1.00 20.24 | AAAA |
| ATOM | 1396 | CD | GLU | 177 | 26.960 | 17.740 | 50.159 | 1.00 27.00 | AAAA |
| | | | | | | | | | |
| MOTA | 1397 | OE | 1 GLU | 177 | 27.974 | 17.935 | 49.450 | 1.00 30.23 | AAAA |
| ATOM | 1398 | OE | 2 GLU | 177 | 25.796 | 17.853 | 49.725 | 1.00 26.89 | AAAA |
| | | | | | | | | | |
| MOTA | 1399 | С | GLU | 177 | 28.284 | 17.713 | 54.376 | 1.00 20.42 | AAAA |
| ATOM | 1400 | 0 | GLU | 177 | 28.486 | 16.503 | 54.527 | 1.00 17.05 | AAAA |
| | | | | | 29.233 | | | 1.00 19.67 | |
| MOTA | 1401 | N | ALA | 178 | | 18.62 6 | 54.527 | | AAAA |
| ATOM | 1402 | CA | ALA | 178 | 30.611 | 18.259 | 54.839 | 1.00 18.18 | AAAA |
| | | | ALA | 178 | 31.464 | 19.519 | 54.918 | 1.00 12.76 | |
| MOTA | 1403 | | | | | | | | AAAA |
| MOTA | 1404 | С | ALA | 178 | 30.806 | 17.418 | 56.106 | 1.00 17.56 | AAAA |
| ATOM | 1405 | 0 | ALA | 178 | 31.690 | 16.555 | 56.167 | 1.00 17.72 | AAAA |
| | | | | | | | | | |
| ATOM | . 14.06 | N | . PHE. | 179 | 29.981 | 17.656 | 57.116 | 1.00 18.82 | AAAA |
| ATOM | 1407 | CA | PHE | 179 | 30.124 | 16.945 | 58.379 | 1.00 20.26 | AAAA |
| | | | | | | | | | |
| MOTA | 1408 | CB | PHE | 179 | 30.554 | 17.948 | 59.439 | 1.00 13.17 | AAAA |
| ATOM | 1409 | CG | PHE | 179 | 31.779 | 18.693 | 59.048 | 1.00 16.28 | AAAA |
| | | | | | | | | | |
| ATOM | 1410 | CD. | 1 PHE | 179 | 31.705 | 20.017 | 58.610 | 1.00 13.77 | AAAA |
| ATOM | 1411 | CD2 | 2 PHE | 179 | 33.002 | 18.031 | 58.995 | 1.00 15.57 | AAAA |
| | 1412 | | 1 PHE | 179 | 32.845 | 20.673 | 58.114 | 1.00 20.03 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 1413 | CE2 | 2 PHE | 179 | 34.145 | 18.677 | 58.500 | 1.00 20.30 | AAAA |
| ATOM | 1414 | CZ | PHE | 179 | 34.060 | 20.002 | 58.058 | 1.00 19.51 | AAAA |
| | | | | | | | | | |
| MOTA. | 1415 | С | PHE | 179 | 28.882 | 16.219 | 58.833 | 1.00 18.52 | AAAA |
| MOTA | 1416 | 0 | PHE | 179 | 28.773 | 15.828 | 60.000 | 1.00 20.21 | AAAA |
| | | | | | | | | | |
| MOTA | 1417 | N | TYR | 180 | 27.969 | 16.016 | 57.895 | 1.00 18.33 | AAAA |
| MOTA | 1418 | CA | TYR | 180 | 26.698 | 15.379 | 58.176 | 1.00 19.93 | AAAA |
| | 1419 | СВ | TYR | 180 | 25.874 | 15.310 | | 1.00 20.97 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 1420 | CG | TYR | 180 | 24.402 | 15.341 | 57.159 | 1.00 19.80 | AAAA |
| ATOM | 1421 | CD1 | TYR | 180 - | 23.565 | 14.337 | 56.686 | 1.00 23.87 | AAAA |
| | | | | | | | | • | |
| ATOM | 1422 | CEI | TYR | 180 | 22.203 | 14.391 | 56.898 | 1.00 21.32 | AAAA |
| ATOM | 1423 | CD2 | TYR | 180 | 23.831 | 16.416 | 57.865 | 1.00 19.02 | AAAA |
| | | | | | | | | | |
| MOTA | 1424 | CEZ | TYR | 180 | 22.470 | 16.482 | 58.084 | 1.00 26.84 | AAAA |
| MOTA | 1425 | CZ | TYR | 180 | 21.659 | 15.462 | 57.594 | 1.00 30.54 | AAAA |
| | 1426 | OH | | . 180 | 20.310 | 15.514 | 57.794 | 1.00 22.81 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 1427 | C | TYR | 180 | 26.855 | 13.970 | 58.737 | 1.00 22.61 | AAAA |
| · ATOM | 1428 | 0 | TYR | 180 | 26.064 | 13.526 | 59.579 | 1.00 23.44 | AAAA |
| | | | | | | | | | |
| ATOM | 1429 | N | ASP | 181 | 27.893 | 13.298 | 58.253 | 1.00 22.27 | AAAA |
| MOTA | 1430 | CA | ASP | 181 | 28.245 | 11.920 | 58.590 | 1.00 33.84 | AAAA |
| | 1431 | CB | ASP | 181 | 28.916 | 11.318 | 57.339 | 1.00 41.74 | AAAA |
| MOTA | | | | | | | | | |
| MOTA | 1432 | CG | ASP | 181 | 30.035 | 10.363 | 57.662 | 1.00 57.71 | AAAA |
| MOTA | 1433 | ODI | ASP | 181 | 30.999 | 10.780 | 58.340 | 1.00 61.40 | AAAA |
| | | | | | | | | 1.00 65.77 | |
| MOTA | 1434 | | ASP | 181 | 29.965 | 9.197 | 57.221 | | AAAA |
| MOTA | 1435 | C | ASP | 181 | 29.107 | 11.654 | 59.838 | 1.00 30.21 | AAAA |
| | 1436 | 0 | ASP | 181 | 29.307 | 10.497 | 60.227 | 1.00 27.84 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 1437 | N | THR | 182 | 29.615 | 12.696 | 60.480 | 1.00 27.53 | AAAA |
| ATOM | 1438 | CA | THR | 182 | 30.472 | 12.466 | 61.634 | 1.00 21.19 | AAAA |
| | | | | | | | | | |
| ATOM | 1439 | CB | THR | 182 | 31.918 | 12.977 | 61.358 | 1.00 26.55 | AAAA |
| ATOM | 1440 | OG1 | THR | 182 | 32.729 | 12.763 | 62.513 | 1.00 25.62 | AAAA |
| | | | | | | | | 1.00 21.67 | |
| ATOM | 1441 | | THR | 182 | 31.922 | 14.471 | 61.037 | | AAAA |
| ATOM | 1442 | C | THR | 182 | 30.010 | 13.050 | 62.954 | 1.00 25.02 | AAAA |
| | 1443 | | | 182 | 29.306 | 14.049 | 62.992 | 1.00 23.56 | AAAA |
| ATOM | | 0 | THR | | | | | | |
| ATOM | 1444 | N | ASP | 183 | 30.434 | 12.424 | 64.042 | 1.00 19.66 | AAAA |
| | 1445 | CA | ASP | 183 | 30.086 | 12.894 | 65.371 | 1,00 21.52 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 1446 | CB | ASP | 183 | 29.735 | 11.700 | 66.275 | 1.00 28.52 | AAAA |
| ATOM | 1447 | CG | ASP | 183 | 30.920 | 10.783 | 66.523 | 100 32.30 | AAAA |
| | | | | | | | | | |
| MOTA | 1448 | OD1 | ASP | 183 | 31.667 | 10.502 | 65.565 | 1.00 30.99 | AAAA |
| MOTA | 1449 | כתס | ASP | 183 | 31.095 | 10.326 | 67.675 | 1.00 48.65 | AAAA |
| | | | | | | | | 1.00 16.66 | AAAA |
| ATOM | 1450 | С | ASP | 183 | 31.257 | 13.685 | 65.947 | 1.00 10.00 | |
| ATOM | 1451 | 0 | ASP | 183 | 31.236 | 14.092 | 67.104. | 1.00 23.37 | AAAA. |
| | | | | 184 | 32.286 | 13.909 | 65.131 | 1.00 21.95 | AAAA |
| MOTA | 1452 | N | GLN | 104 | JZ.200 | ±0.303 | | | , inner |
| · · · · · · · · · · · · · · · · · · · | | | | • | | | | | • |

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Figure 16-23

| | ATOM | 1453 | CA | GLN | 184 | 3 | 33.437 | 14.672 | 65.590 | 1.00 | 17.65 | AAA | Δ |
|---|--------|------|-----|-------|-------|-----|--------|--------|--------|-------|-------|--------------|----|
| | ATOM | 1454 | | | 184 | | 34.701 | | | | | | |
| | | | | | | | | | | | 21.36 | AAA | |
| | ATOM | 1455 | | | 184 | | 35.068 | | | | 27.38 | AAA | |
| | MOTA | 1456 | CD | GLN | 184 | 3 | 36.485 | 12.476 | 64.691 | 1.00 | 31.96 | AAA | A |
| | MOTA | 1457 | OE | 1 GLN | 184 | 3 | 36.899 | 12.760 | 63.573 | 1.00 | 29.90 | AAA | A |
| | ATOM | 1458 | NE | 2 GLN | 184 | | 37.239 | | | | 31.84 | AAA | |
| | | 1459 | | | | | | | | | | | |
| | ATOM | - | | GLN | 184 | | 33.207 | | | | 18.54 | AAA | |
| | ATOM | 1460 | 0 | GLN | 184 | 3 | 33.881 | 17.009 | | 1.00 | 18.11 | AAA | A |
| | ATOM | 1461 | N | VAL | 185 | 3 | 2.258 | 16.481 | 64.519 | 1.00 | 19.18 | AAA | A |
| | MOTA | 1462 | CA | VAL | 185 | | 1.934 | | | | 21.57 | AAA | |
| | ATOM | 1463 | CB | | 185 | | 2.261 | | | | | | |
| | | | | | | | | | | | 22.64 | AAA | |
| | ATOM | 1464 | | 1 VAL | 185 | | 1.994 | | | | 16.26 | AAA A | Ą |
| | MOTA | 1465 | CG. | 2 VAL | 185 | 3 | 3.722 | 17.924 | 62.500 | 1.00 | 16.77 | AAA | A |
| | ATOM | 1466 | С | VAL | 185 | 3 | 0.449 | 18.035 | 64.523 | | 15.91 | AAA | |
| | ATOM | 1467 | 0 | VAL | 185 | | 9.658 | | | | 20.79 | | |
| | | | | | | | | | | | | LAAA | |
| | ATOM | 1468 | N | PHE | | | 0.081 | | | | 18.73 | AAA | |
| | ATOM | 1469 | CA | PHE | 186 | 2 | 8.687 | 19.446 | 65.435 | 1.00 | 16.22 | AAA | Ą |
| | ATOM | 1470 | CB | PHE | 186 | 2 | 8.432 | 19.559 | 66.952 | 1.00 | 16.83 | AAAA | A |
| | . ATOM | 1471 | CG | PHE | 186 | . 2 | 6.976 | 19.682 | 67.299 | | 17.96 | , AAA | |
| | ATOM | 1472 | | 1 PHE | 186 | | 6.319 | | 67.968 | | | | |
| | | | | | | | | | | | 23.24 | AAA | |
| | MOTA | 1473 | | 2 PHE | 186 | | 6.240 | | 66.904 | | 15.41 | AAAA | |
| | ATOM | 1474 | CE: | l PHE | 186 | 2 | 4.953 | 18.738 | 68.235 | 1.00 | 18.99 | AAA | A |
| | MOTA | 1475 | CE | PHE S | 186 | 2 | 4.879 | 20.887 | 67.168 | 1.00 | 24.05 | AAA | A |
| | ATOM | 1476 | CZ | PHE | 186 | | 4.234 | | 67.838 | | 22.93 | AAA | |
| | | 1477 | | PHE | 186 | | | | | | | | |
| | ATOM | | C | | | | 8.437 | | 64.778 | | 17.16 | AAA | |
| | ATOM | 1478 | 0 | PHE | 186 | | 9.192 | | 64.993 | | 19.37 | AAA | |
| | ATOM | 1479 | N | VAL | 187 | 2 | 7.391 | 20.874 | 63.961 | 1.00 | 19.67 | AAAA | 4 |
| | MOTA | 1480 | CA | VAL | 187 | 2 | 7.075 | 22.116 | 63.277 | 1.00 | 17.74 | AAA | 4 |
| | ATOM | 1481 | CB | VAL | 187 | | 7.010 | | 61.720 | | 18.65 | AAAA | |
| | ATOM | 1482 | | VAL | 187 | | 6.578 | | 61.024 | | | | |
| | | | | | | | | | | | 17.31 | AAAA | |
| | ATOM | 1483 | | VAL | | | 8.359 | | 61.194 | | 16.65 | AAAA | |
| | ATOM | 1484 | С | VAL | 187 | 2 | 5.732 | 22.637 | 63.746 | 1.00 | 18.46 | AAA A | ¥ |
| • | MOTA | 1485 | 0 | VAL | 187 | 2 | 4.752 | 21.903 | 63.764 | 1.00 | 20.64 | AAA | À. |
| | ATOM | 1486 | N | LEU | 188 | | 5.708 | | 64.150 | | 14.42 | LAAA | |
| | ATOM | 1487 | ĊA | LEU | 188 | | 4.482 | 24.563 | 64.567 | | 16.68 | AAAA | |
| | | | | | | | | - | | | | | |
| | ATOM | 1488 | CB | LEU | 188 | | 4.568 | 25.070 | 66.009 | | 13.98 | LAAA | |
| | MOTA | 1489 | CG | LEU | 188 | 2. | 3.522 | 26.119 | 66.450 | 1.00 | 13.66 | · AAAA | |
| | ATOM | 1490 | CD1 | LEU | 188 | 2: | 2.103 | 25.556 | 66.401 | 1.00 | 15.55 | AAAA | 4 |
| | ATOM | 1491 | CD2 | LEU | 188 | 2 | 3.844 | 26.585 | 67.861 | | 16.40 | AAAA | |
| | ATOM | 1492 | C | LEU | 188 | | 4.272 | 25.756 | 63.667 | | 20.01 | AAAA | |
| | | | | | | | | | | | | | |
| | ATOM | 1493 | 0 | LEU | 188 | | 5.164 | 26.595 | 63.506 | | 18.86 | AAAA | |
| | MOTA | 1494 | N | SER | 189 | 2. | 3.106 | 25.845 | 63.057 | .1.00 | 14.46 | AAAA | ١ |
| | ATOM | 1495 | CA | SER | 189 | 2: | 2.841 | 27.011 | 62.230 | 1.00 | 14.56 | AAAA | 1 |
| | ATOM | 1496 | CB | SER | 189 | 2: | 2.896 | 26.668 | 60.737 | 1.00 | 15.55 | AAAA | |
| | ATOM | 1497 | OG | SER | 189 | | 2.619 | 27.851 | 60.008 | | 14.09 | AAAA | |
| | | | | | | | | | | | | | |
| | ATOM | 1498 | Ç | SER | 189 | | 1.487 | 27.606 | 62.508 | | 15.24 | AAAA | |
| _ | MOTA | 1499 | 0 | SER | 189 | | 0.509 | 26.885 | 62.578 | 1.00 | 21.46 | AAAA | k. |
| | ATOM | 1500 | N | LEU | 190 | 2: | 1.423 | 28.921 | 62.690 | 1.00 | 14.92 | AAAA | L. |
| | MOTA | 1501 | CA | LEU | 190 | 20 | 0.128 | 29.572 | 62.826 | 1.00 | 15.54 | AAAA | ı. |
| | ATOM | 1502 | CB | LEU | 190 | | 0.084 | 30.663 | 63.906 | | 21.02 | AAAA | |
| | | | | | | | | | | | | | |
| | ATOM | 1503 | | LEU | 190 | | | | 65.339 | 1.00 | | AAAA | |
| | ATOM | 1504 | CDI | LEU | 190 | | | 31.437 | 66.210 | | 19.75 | AAAA | L |
| | ATOM | 1505 | CD2 | LEU | 190 | 20 |).547 | 29.130 | 65.831 | 1.00 | 19.08 | AAAA | L |
| | MOTA | 1506 | С | LEU | 190 · | 20 | 1.035 | 30.250 | 61.456 | 1.00 | 14.31 | AAAA | |
| | | 1507 | ō | LEU | 190 | | | 30.752 | 60.951 | | 15.43 | AAAA | |
| | MOTA | | | | | | | | | | | | |
| | ATOM | 1508 | | HIS | 191 | | 3.855 | 30.285 | 60.856 | | 16.88 | AAAA | |
| | MOTA | 1509 | CA | HIS | 191 | 18 | 3.732 | 30.884 | 59.535 | 1.00 | 14.34 | AAAA | |
| | ATOM | 1510 | CB | HIS | 191 | 19 | 9.506 | 30.015 | 58.539 | 1.00 | 17.34 | AAAA | |
| | ATOM | 1511 | CG | HIS | 191 | | 229 | 28.546 | 58.697 | | 14.27 | AAAA | |
| | | | | HIS | 191 | | 9.941 | | | | | | |
| | ATOM | 1512 | | | | | | 27.578 | 59.319 | | 9.60 | AAAA | |
| | ATOM | 1513 | | HIS | 191 | | 3.073 | 27.940 | 58.247 | | 21.22 | AAAA | |
| | ATOM | 1514 | CE1 | HIS | 191 | 18 | 3.088 | 26.660 | 58.582 | 1.00 | 17.22 | AAAA | |
| | ATOM | 1515 | | HIS | 191 | | 212 | 26.415 | 59.232 | | 20.70 | AAAA | |
| | | 1516 | C | HIS | 191 | | 7.277 | 31.026 | 59.110 | | 16.19 | AAAA | |
| | ATOM | | | | | | | | | | | | |
| | ATOM | 1517 | 0 | HIS | 191 | | | 30.489 | 59.766 | | 16.73 | AAAA | |
| | ATCM · | 1518 | N | GLN | 192 | 17 | 7.044 | 31.796 | 58.045 | 1.00 | 14.78 | AAAA | |
| | • | | • | | | | | | - | | | • | |
| | | | | | • | | | | | | | | |
| | | | | | | | | | | | | | |

Figure 16-24

| | | | | - | | | | | |
|-------|-------|------|--------|-------|----------|--------|--------|-------------|------|
| MOTA | 151 | 9 C | A GLM | 1 192 | 15.683 | 31.968 | 57.516 | 1.00 16.33 | KAAA |
| ATOM | 152 | 0 C | B GLN | | 15.669 | | | | |
| ATOM | 152 | | | | 16.174 | | | | AAAA |
| | | | | | | | | | AAAA |
| MOTA | 152 | | | | 16.408 | | | 1.00 14.74 | AAAA |
| MOTA | 152 | | El GLN | 192 | 15.490 | 35.566 | 54.587 | 1.00 20.46 | AAAA |
| ATOM | . 152 | 4 NI | E2 GLN | 192 | 17.630 | 34.839 | 54.665 | | AAAA |
| MOTA | 152 | 5 C | GLN | 192 | 15.262 | | | | |
| ATOM | 152 | | GLN | | 16.071 | | | | AAAA |
| | 152 | | | | | | _ | | AAAA |
| AŢOM | | | SER | | 14.007 | | | 1.00 15.63 | AAAA |
| ATOM | 152 | | - | | 13.561 | 28.907 | 56.877 | 1.00 13.84 | AAAA |
| ATOM | 1529 | 9 CE | SER | 193 | 12.097 | 28.677 | 57.284 | 1.00 17.28 | AAAA |
| ATOM | 1530 | 000 | SER | 193 | 11.639 | 27.439 | | 1.00 17.58 | |
| ATOM | 1531 | L C | SER | • | - 13.687 | | | -1.00 11.80 | AAAA |
| ATOM | 1532 | | SER | | | | | | AAAA |
| | | | | | 13.400 | | | 1.00 18.44 | AAAA |
| MOTA | 1533 | | PRO | | 14.103 | | | 1.00 14.59 | AAAA |
| ATOM | 1534 | | PRO | 194 | 14.335 | 26.325 | 55.782 | 1.00 19.22 | AAAA |
| MOTA | 1535 | 5 CA | PRO | 194 | 14.268 | 27.143 | 53.513 | 1.00 15.30 | AAAA |
| ATOM | 153€ | CB | PRO | 194 | 14.892 | 25.737 | | 1.00 18.33 | |
| ATOM | 1537 | | | 194 | 15.359 | | | | AAAA |
| ATOM | 1538 | | | | | | | 1.00 22.34 | AAAA |
| | | | PRO | 194 | 12.880 | | | 1.00 16.40 | AAAA |
| MOTA | 1539 | | PRO | 194 | 12.757 | | 51.640 | 1.00 19.43 | AAAA |
| MOTA | 1540 | N | GLU | 195 | 11.828 | 27.151 | 53.681 | 1.00 20.57 | AAAA |
| ATOM | 1541 | . CA | GLU | 195 | 10.483 | 27.161 | 53.099 | 1.00 30.15 | AAAA |
| ATOM | 1542 | CB | GLU | 195 | 9.386 | 27.037 | | 1.00 31.91 | |
| ATOM | 1543 | | GLU | 195 | 8.987 | 28.325 | | | |
| ATOM | 1544 | | | 195 | | | | 1.00 45.60 | AAAA |
| | | | | | 7.880 | 29.119 | | 1.00 34.45 | AAAA |
| ATOM | 1545 | | 1 GLU | 195 | 7.635 | 30.259 | | 1.00 43.98 | AAAA |
| MOTA | 1546 | | 2 GLU | 195 | . 7.241 | 28.627 | 53.210 | 1.00 38.39 | AAAA |
| ATOM | 1547 | С | GLU | 195 | 10.333 | 28.474 | 52.318 | 1.00 26.92 | AAAA |
| ATOM | 1548 | 0 | GLU | 195 | 9.522 | 28.557 | 51.395 | 1.00 24.59 | AAAA |
| ATOM | 1549 | N | TYR | 196 | 11.116 | 29.501 | 52.669 | 1.00 18.16 | AAAA |
| MOTA | 1550 | CA | TYR | 196 | 11.024 | 30.753 | 51.922 | | |
| ATOM | 1551 | CB | TYR | 196 | | | | 1.00 15.81 | AAAA |
| | | | | | 10.208 | 31.801 | 52.690 | 1.00 20.01 | AAAA |
| ATOM | 1552 | CG | TYR | 196 | 10.868 | 32.353 | 53.932 | 1.00 19.77 | AAAA |
| ATOM | 1553 | CD | | 196 | 11.779 | 33.408 | 53.853 | 1.00 18.24 | AAAA |
| ATOM | 1554 | | L TYR | 196 | 12.407 | 33.898 | 54.988 | 1.00 18.50 | AAAA |
| ATOM | 1555 | CD2 | TYR | 196 | 10.598 | 31.801 | 55.185 | 1.00 18.12 | AAAA |
| ATOM | 1556 | CE2 | TYR | 196 | 11.223 | 32.283 | 56.339 | 1.00 21.09 | AAAA |
| ATOM | 1557 | CZ | TYR | 196 | 12.125 | 33.326 | 56.235 | | |
| ATOM | 1558 | ОН | TYR | 196 | | | | 1.00 20.39 | AAAA |
| | | | | | 12.759 | 33.784 | 57.367 | 1.00 16.20 | AAAA |
| ATOM | 1559 | Ç | TYR | 196 | 12.342 | 31.372 | 51.475 | 1.00 16.89 | AAAA |
| ATOM | 1560 | 0 | TYR | 196 | 12.336 | 32.347 | 50.718 | 1.00 23.08 | AAAA |
| MOTA | 1561 | N | ALA | 197 | 13.466 | 30.817 | 51.911 | 1.00 17.52 | AAAA |
| ATOM | 1562 | CA | ALA | 197 | 14.754 | 31.400 | 51.512 | 1.00 20.26 | AAAA |
| ATOM | 1563 | CB | ALA | 197 | 15.315 | 32.261 | 52.659 | 1.00 20.74 | AAAA |
| ATOM | 1564 | С | ALA | 197 | 15.814 | 30.392 | 51.074 | 1.70 13.51 | |
| ATOM | 1565 | ō | ALA | 197 | 15.787 | | | | AAAA |
| ATOM | 1566 | N | | | | 29.229 | 51.457 | 1 00 19.35 | AAAA |
| | | | PHE | 198 | 16.757 | 30.869 | 50.257 | 1. 70 18.01 | AAAA |
| ATOM | 1567 | CA | PHE | 198 | 17.861 | 30.049 | 49.782 | 1.00 17.97 | AAAA |
| ATOM | 1568 | CB | PHE | 198 | 18.929 | 30.933 | 49.119 | 1.00 20.38 | AAAA |
| ATOM | 1569 | CG | PHE | 198 | 20.094 | 30.162 | 48.545 | 1.00 23.61 | AAAA |
| ATOM | 1570 | CD1 | PHE | 198 | 20.039 | 29.660 | 47.245 | 1.00 29.71 | AAAA |
| MOTA | 1571 | | PHE | 198 | 21.229 | 29.899 | | | |
| ATOM | 1572 | | PHE | 198 | | | 49.321 | 1.00 19.06 | AAAA |
| | | | | | 21.091 | 28.908 | 46.719 | 1.00 30.39 | AAAA |
| ATOM | 1573 | CE2 | | 198 | 22.290 | 29.145 | 48.807 | 1.00 23.17 | AAAA |
| MOTA | 1574 | CZ | PHE | 198 | 22.218 | 28.646 | 47.493 | 1.00 22.74 | AAAA |
| ATOM | 1575 | С | PHE | 198 | 18.453 | 29.419 | 51.032 | 1.00 16.02 | AAAA |
| ATOM | 1576 | 0 | PHE | 198 | 18.552 | 30.073 | 52.061 | 1.00 20.95 | AAAA |
| ATOM | 1577 | N | PRO | 199 | 18.941 | 28.176 | 50.937 | | |
| | 1578 | | | | | | | 1.00 19.92 | AAAA |
| MOTA | | CD | PRO | 199 | 19.600 | 27.508 | 52.074 | 1.00 17.86 | AAAA |
| ATOM | 1579 | CA | PRO | 199 | 18.990 | 27.318 | 49.744 | 1.00 23.54 | AAAA |
| MOTA | 1580 | CB | PRO | 199 | 20.108 | 26.344 | 50.095 | 1.00 22.70 | AAAA |
| MOTA | 1581 | CG | PRO | 199 | 19.813 | 26.087 | 51.534 | 1.00 23.16 | AAAA |
| | 1582 | С | PRO | 199 | 17.710 | 26.595 | 49.312 | 1.00 30.97 | AAAA |
| ATOM | 1583 | ō | PRO | 199 | 17.733 | 25.855 | 48.322 | 1.00 23.25 | |
| ATOM | 1584 | | PHE | 200 | | | | | AAAA |
| ATOM. | 1000 | N | rns | 200 | 16.621 | 26.795 | 50.054 | 1.00 20.32 | AAAA |

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| ATOM | 1585 | CA | PHE | 200 | 15.319 | 26.166 | 49.752 | 1.00 20.27 | AAAA |
|--------|------|-----|-----|-------------|----------------|--------|---------|------------|--------|
| | 1586 | CB | PHE | 200 | 14.840 | 26.533 | 48.346 | 1.00 19.77 | AAAA |
| MOTA | | | _ | | | | | | |
| ATOM | 1587 | CG | PHE | 200 | 14.752 | 27.999 | 48.082 | 1.00 18.06 | AAAA |
| ATOM | 1588 | CDI | PHE | 200 | 15.742 | 28.644 | 47.346 | 1.00 18.97 | AAAA |
| | | | | | | | | 1.00 19.06 | |
| MOTA | 1589 | CDZ | PHE | 200 | 13.654 | 28.736 | 48.519 | | AAAA |
| ATOM | 1590 | CE1 | PHE | 200 | 15.635 | 30.003 | 47.042 | 1.00 21.67 | AAAA |
| | | | | | | 30.101 | 48.221 | 1.00 22.60 | |
| ATOM | 1591 | CEZ | PHE | 200 | 13.539 | | | | AAAA |
| ATOM | 1592 | CZ | PHE | 200 | 14.527 | 30.736 | 47.482 | 1.00 18.93 | AAAA |
| | | | | | | | 49.845 | 1.00 18.44 | |
| ATOM | 1593 | С | PHE | 200 | 15.294 | 24.637 | | | AAAA |
| ATOM | 1594 | 0 | PHE | 200 | 14.302 | 24.049 | 50.272 | 1.00 20.74 | AAAA |
| | | | | 201 | 16.384 | 24.004 | 49.418 | 1.00 20.77 | AAAA |
| ATOM | 1595 | N | GLU | | | | | | |
| MOTA | 1596 | CA | GLU | 201 | 16.522 | 22.542 | 49.399 | 1.00 27.34 | AAAA |
| | | CB | GLU | 201 | 17.498 | 22.146 | 48.284 | 1.00 28.99 | AAAA |
| MOTA | 1597 | | | | | | | | |
| ATOM | 1598 | CG | GLU | 201 | 17.024 | 22.458 | 46.881 | 1.00 34.82 | AAAA |
| ATOM | 1599 | CD | GLU | 201 | 18.123 | 22.265 | 45.848 | 1.00 32.40 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 1600 | OE1 | GLU | 201 | 18.70 1 | 21.155 | 45.769 | 1.00 38.28 | AAAA |
| | 1601 | OF2 | GLU | 201 | 18.405 | 23.230 | 45.111 | 1.00 40.08 | AAAA |
| ATOM | | | | | | | | | |
| · ATOM | 1602 | С | GLU | 201 | 17.007 | 21.891 | 50.695 | 1.00 23.51 | AAAA |
| ATOM | 1603 | 0 | GLU | 201 | 16.845 | 20.689 | 50.886 | 1.00 23.17 | AAAA |
| | | | | | 17.619 | 22.681 | 51.571 | 1.00 20.03 | AAAA |
| MOTA | 1604 | N | LYS | 202 | | | | | |
| MOTA | 1605 | CA | LYS | 202 | 18.178 | 22.177 | 52.829 | 1.00 17.01 | AAAA |
| | •_ | CB | LYS | 202 | 19.666 | 21.862 | 52.634 | 1.00 19.24 | AAAA |
| ATOM | 1606 | | | | | | | | |
| ATOM | 1607 | CG | LYS | 202 | 19.903 | 20.769 | 51.611 | 1.00 36.04 | AAAA |
| | 1608 | CD | LYS | 202 | 20.99 7 | 21.162 | 50.648 | 1.00 45.11 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 1609 | CE | LYS | 202 | 21.060 | 20.209 | 49.463 | 1.00 55.83 | AAAA |
| ATOM | 1610 | NZ | LYS | 202 | 22.024 | 20.662 | 48.422 | 1.00 28.09 | AAAA |
| | | | | | | | 53.899 | 1.00 17.02 | AAAA |
| ATOM | 1611 | С | LYS | 2 02 | 18.016 | 23.240 | | | |
| MOTA | 1612 | 0 | LYS | 202 | . 17.705 | 24.381 | 53.585 | 1.00 20.20 | AAAA |
| | | | GLY | 203 | 18.232 | 22.875 | 55.160 | 1.00 22.94 | AAAA |
| MOTA | 1613 | N | | | | | | | |
| MOTA | 1614 | CA | GLY | 203 | 18.064 | 23.850 | 56.223 | 1.00 19.38 | AAAA |
| | 1615 | С | GLY | 203 | 16.874 | 23.564 | 57.128 | 1.00 20.48 | AAAA |
| MOTA | | | | | | | | 1.00 18.55 | AAAA |
| MOTA | 1616 | 0 | GLY | 203 | 16.607 | 24.312 | 58.070 | | |
| ATOM | 1617 | N | PHE | 204 | 16.150 | 22.484 | 56.852 | 1.00 15.42 | AAAA |
| | | | | 204 | 14.983 | 22.143 | 57.670 | 1.00 20.73 | AAAA |
| MOTA | 1618 | CA | PHE | | | | | | |
| MOTA | 1619 | CB | PHE | 204 | 14.018 | 21.212 | 56.903 | 1.00 19.97 | AAAA |
| | 1620 | CG | PHE | 204 | 13.441 | 21.838 | 55.667 | 1.00 19.63 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 1621 | CDI | PHE | 204 | 14.137 | 21.801 | 54.459 | 1.00 24.96 | AAAA |
| ATOM | 1622 | CD2 | PHE | 204 | 12.230 | 22.523 | 55.725 | 1.00 18.92 | AAAA |
| | | | | | 13.636 | 22.438 | 53.327 | 1.00 20.66 | AAAA |
| MOTA | 1623 | | PHE | 204 | | | | | |
| ATOM | 1624 | CE2 | PHE | 204 | 11.720 | 23.169 | 54.597 | 1.00 24.86 | AAAA |
| | 1625 | CZ | PHE | 204 | 12.422 | 23.127 | 53.400 | 1.00 23.66 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 1626 | Ç | PHE | 204 | 15.376 | 21.513 | 59.006 | 1.00 18.73 | AAAA |
| ATOM | 1627 | 0 | PHE | 204 | 1.6.415 | 20.851 | 59.131 | 1.00 20.18 | AAAA |
| | | | | | | 21.726 | 59.994 | 1.00 19.46 | AAAA |
| ATOM | 1628 | N | LEU | 205 | 14.518 | | | | |
| MOTA | 1629 | CA | LEU | 205 | 14.727 | 21.244 | 61.356 | 1.00 21.09 | AAAA |
| | | | LEU | 205 | 13.547 | 21.674 | 62.233 | 1.00 23.44 | · AAAA |
| MOTA | 1630 | CB | | | | | | | |
| ATOM | 1631 | CG | LEU | 205 | 13.506 | 21.222 | 63.693 | 1.00 23.23 | AAAA |
| | 1632 | CD1 | LEU | 205 | 14.717 | 21.736 | 64.445 | 1.00 24.06 | AAAA |
| MOTA | | | | | 12.224 | 21.743 | 64.312 | 1.00 30.63 | AAAA |
| ATOM | 1633 | CDZ | LEU | 205 | | | | | |
| ATOM | 1634 | С | LEU | 205 | 14.943 | 19.748 | 61.489 | 1.00 23.53 | AAAA |
| | | | | 205 | 15.659 | 19.315 | 62.381 | 1.00 21.28 | AAAA |
| ATOM | 1635 | 0 | LEU | | | | | | |
| ATOM | 1636 | N | GLU | 206 | 14.356 | 18.959 | 60.591 | 1.00 21.59 | AAAA |
| | | CA | GLU | 206 | 14.487 | 17.502 | 60.686 | 1.00 27.89 | AAAA |
| ATOM | 1637 | | | | | | | | AAAA |
| ATOM · | 1638 | CB | GLU | 206 | 13.345 | 16.816 | 59.928 | 1.00 28.90 | |
| | 1639 | CG | GLU | 206 | 12.060 | 17.615 | 59.942 | 1.00 48.55 | AAAA |
| MOTA | | | | | | 18.832 | 59.042 | 1.00 46.86 | AAAA |
| ATOM | 1640 | CD | GLU | 206 | 12.169 | | | | |
| ATOM | 1641 | OE1 | GLU | 206 | 11.360 | 19.769 | 59.178 | 1.00 21.58 | AAAA |
| | | | | 206 | 13.076 | 18.833 | 58.181 | 1.00 63.58 | AAAA |
| MOTA | 1642 | | GLU | | | | | | |
| ATOM | 1643 | С | GLU | 206 | 15.819 | 16.955 | 60.188 | 1.00 22.86 | AAAA |
| | | | GLU | 206 | 16.071 | 15.753 | 60.286 | 1.00 21.21 | AAAA |
| ATOM | 1644 | 0 | | | | | | | |
| ATOM | 1645 | N | GLU | 207 | 16.666 | 17.816 | 59.631 | 1.00 25.04 | AAAA |
| | | CA | GLU | 207 | 17.976 | 17.373 | 59.152 | 1.00 19.61 | AAAA |
| ATOM | 1646 | | | | | | | 1.00 20.75 | AAAA |
| ATOM | 1647 | CB | GLU | 207 | 18.483 | 18.322 | 58.055 | | |
| | 1648 | CG | GLU | 207 | 17.682 | 18.222 | 56.753 | 1.00 18.44 | AAAA |
| ATOM | | | | | _ | | 55.983 | 1.00 24.75 | AAAA |
| MOTA | 1640 | CD | GLU | 207 | 17.687 | 19.514 | | | |
| | 1649 | | | | | 22 122 | EE 0.40 | | |
| | | OE1 | GLU | 207 | 18.738 | 20.18Z | 55.948 | 1.00 22.17 | AAAA |
| MOTA | 1650 | OE1 | GLU | 207 | 18.738 | 20.182 | 55.548 | 1.00 22.17 | |
| | | OE1 | GLU | 207 | 18.738 | 20.182 | 55.546 | 1.00 22.17 | * |

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| | ATO | | 51 | OE2 GI | בַ ט 207 | 16.6 | 46 19.8 | 54 55.39 | 6 1 00 15 50 | |
|----|--------------|--------------|----------|----------------|-----------------|------------------|------------------|------------------|--------------------------|--------------|
| | ATO | | 52 | C . CĪ | JU 207 | 18.9 | | | | AAAA |
| | ATOM | | | 0 GI | | 19.50 | | | | AAAA |
| | ATOM | | | N II | | 19.08 | | 18 60.98 | | AAAA |
| | ATOM | | _ | CA II | | 19.93 | | | 3 1.00 22.37 | AAAA |
| ٠. | ATOM | | | CB II | | 19.11 | | 52 63.40 | | AAAA AAAA |
| | ATOM | | | CG2 IL | | 19.9€ | | 3 64.65 | | AAAA |
| | ATOM ATOM | | | CG1 IL | | 17.90 | | 51 53.625 | 1.00 21.61 | AAAA |
| | ATOM | | | CD1 IL C IL | | 17.02 | | | 1.00 41.40 | AAAA |
| | ATOM | | | C IL | | 21.15 | | | 1.00 24.74 | AAAA |
| | ATOM | | | N CL | | 21.78 | _ | | 1.00 22.68 | AAAA |
| | ATOM | | | CA GL | | 21.51 | | | | AAAA |
| | ATOM | | | GL. GL | | 22.69 | | | | AAAA |
| | ATOM | | | | | 22.34 21.16 | | | | AAAA |
| | ATOM | | | | | 23.37 | | | | AAAA |
| | MOTA | 166 | 57 (| A GLI | | 23.23 | | | | AAAA |
| | ATOM | 166 | 68 C | B GL | | 23.40 | | | | AAAA |
| | ATOM | 166 | 59 C | G GLU | | 23.04 | | | | AAAA |
| | ATOM | 167 | '0 C | D GLU | | 23.17 | 0 9.95 | | | AAAA |
| | MOTA | 167 | | El GLU | 210 | 24.29 | | | 1.00 65.37 1.00 62.00 | AAAA |
| | MOTA | 167 | | E2 GLU | 210 | 22.15 | 3 9.89 | 4 54.768 | 1.00 62.00 | AAAA |
| | ATOM | 167 | | | | 24.329 | 9 9.70 | | 1.00 73.24 | AAAA |
| | ATOM | 167 | | | | 25.44 | | | 1.00 28.85 | AAAA |
| | ATOM | 167 | | | | 24.012 | | 1 60.121 | 1.00 27.84 | AAAA AAAA |
| | MOTA MOTA | 167 | | | | 24.991 | | 2 60.657 | 1.00 26.25 | AAAA |
| | ATOM | 167 167 | | GLY | | 25.545 | | | 1.00 27.79 | AAAA |
| | ATOM | 167 | | | 211 212 | 24.788 | | | 1.00 28.66 | AAAA |
| | ATOM | 168 | | | | 26.865 | | 62.150 | 1.00 34.62 | AAAA . |
| | ATOM | 168 | | | 212 | 27.512 29.029 | | | 1.00 34.39 | AAAA |
| | MOTA | 1682 | | | 212 | 29.505 | | 63.273 | 1.00 40.40 | AAAA |
| | ATOM | 1683 | cr | | 212 | 29.139 | 5.770 | | 1.00 53.97 | AAAA |
| | ATOM | 1684 | CE | | 212 | 29.612 | | | 1.00 61.93 | AAAA |
| | ATOM | 1685 | | LYS | 212 | 31.091 | | 63.711 | 1.00 62.74 1.00 70.11 | AAAA |
| | ATOM | 1686 | _ | LYS | 212 | 27.181 | 9.741 | | 1.00 36.04 | AAAA |
| | ATOM | 1687 | | LYS | 212 | 27.109 | 10.126 | | 1.00 28.34 | AAAA |
| | ATOM | 1688 | | GLY | 213 | 26.959 | 10.543 | | 1.00 31.47 | AAAA AAAA |
| | MOTA MOTA | 1689 | | | 213 | 26.648 | 11.948 | | 1.00 31.68 | AAAA |
| | ATOM ATOM | 1690 1691 | | GLY | 213 | 25.189 | 12.291 | 63.142 | 1.00 28.78 | AAAA |
| | MOTA | 1692 | | GLY LYS | 213 | 24.840 | 13.460 | 63.259 | 1.00 22.56 | AAAA |
| | MOTA | 1693 | | | 214 214 | 24.317 | 11.292 | 63.222 | 1.00 28,54 | AAAA |
| | MOTA | 1694 | | | 214 | 22.905 22.080 | 11.585 | 63.463 | 1.00 31.11 | AAAA |
| | MOTA | 1695 | | LYS | 214 | 20.583 | 10.295 10.461 | 63.325 | 1.00 31.03 | AAAA |
| ž | MOTA | 1696 | CD | LYS | 214 | 19.968 | 9.115 | 63.224 | 1.00 38.15 | AAAA |
| ; | MOT | 1697 | CE | LYS | 214 | 18.490 | 9.220 | 62.844 62.537 | 1.00 40.49 | AAAA |
| | MOT | 1698 | NZ | LYS | 214 | 17.927 | 7.924 | 62.064 | 1.00 48.02 1.00 44.99 | AAAA |
| | MOTA | 1699 | С | LYS | 214 | 22.834 | 12.160 | 64.875 | 1.00 24.99 | AAAA |
| | MOTA | 1700 | 0 | LYS | 214 | 23.260 | 11.524 | 65.831 | 1.00 33.33 | AAAA |
| | MOT | 1701 | N | GLY | 215 | 22.310 | 13.376 | 64.997 | 1.00 24.38 | AAAA AAAA |
| | TOM | 1702 | CA | GLY | 215 | 22.230 | 14.034 | 66.290 | 1.00 26.03 | AAAA |
| | TOM | 1703 | C | GLY | 215 | 23.298 | 15.115 | 66.447 | 1.00 27.03 | AAAA |
| | TOM TOM | 1704 1705 | 0 | GLY | 215 | 23.352 | 15.820 | 67.458 | 1.00 23.34 | AAAA |
| | TOM | 1705 | N | TYR | 216 | 24.152 | 15.260 | 65.439 | 1.00 22.79 | AAAA |
| | TOM | 1707 | CA CB | TYR | 216 | 25.217 | 16.257 | 65.512 | 1.00 25.51 | AAAA |
| | TOM | 1708 | CG | TYR TYR | 216 | 26.592 | 15.576 | 65.406 | 1.00 20.54 | AAAA |
| | TOM | 1709 | | TYR | 216 216 | 26.900 26.221 | 14.671 | | 1.00 26.47 | AAAA |
| | TOM | 1710 | | TYR | 216 | | 13.464 | 66.757 | 1.00 28.96 | AAAA |
| | TOM | 1711 | | TYR | 216 | 26.455 27.832 | 12.660 | | 1.00 33.08 | AAAA |
| | TOM | 1712 | CE2 | TYR | 216 | 28.074 | 15.052 | 67.552 | 1.00 24.21 | AAAA |
| | | 1713 | CZ | TYR | 216 | 27.378 | 14.254 13.063 | | 1.00 34.45 | AAAA |
| | | 1714 | он | TYR | 216 | 27.580 | 12.291 | | 1.00 40.53 | AAAA |
| | | 1715 | С | TYR | 216 | 25.104 | 17.391 | ~ A A | 1.00 45.67 | AAAA |
| | | 1716 | 0 | TYR | 216 | 26.097 | 18.014 | | 1.00 22.57 | AAAA |
| | | | | | • . | | | - | 1.00 19.70 | AAAA |
| | | • | | | | | | | | • |

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| | | | | | | | | 1 00 00 00 | |
|--------|-------|-----|-----|-------|----------|--------|---------|------------|------|
| ATOM | 1717 | N | ASN | 217 | 23.889 | 17.635 | 64.027 | 1.00 22.88 | AAAA |
| ATOM | 1718 | CA | ASN | 217 | 23.621 | 18.729 | 63.109 | 1.00 22.60 | AAAA |
| ATOM | 1719 | CB | ASN | 217 | 23.453 | 18.240 | 61.671 | 1.00 16.61 | AAAA |
| | 1720 | CG | ASN | 217 | 23.233 | 19.387 | 60.695 | 1.00 17.16 | AAAA |
| MOTA | 1721 | OD1 | | 217 | 22.098 | 19.704 | 60.307 | 1.00 20.23 | AAAA |
| MOTA | | | | 217 | 24.320 | 20:032 | 60.309 | 1.00 12.18 | AAAA |
| MOTA | 1722 | ND2 | | | 22.311 | 19.296 | 63.630 | 1.00 17.65 | AAAA |
| MOTA | 1723. | C | ASN | 217 | 21.381 | 18.550 | 63.894 | 1.00 17.63 | AAAA |
| MOTA | 1724 | 0 | ASN | 217 | | | 63.793 | 1.00 21.68 | AAAA |
| MOTA | 1725 | N | LEU | 218 | 22.236 | 20.610 | | 1.00 21.20 | AAAA |
| MOTA | 1726 | CA | LEU | 218 | 21.014 | 21.197 | 64.320 | | AAAA |
| ATOM | 1727 | CB | LEU | 218 | - 21.186 | 21.547 | 65.808 | 1.00 17.73 | |
| ATOM | 1728 | CG | LEU | 218 | 19.906 | 21.702 | 66.647 | 1.00 32.30 | AAAA |
| MOTA | 1729 | CD1 | | 218 | 20.228 | 22.427 | 67.944 | 1.00 24.51 | AAAA |
| MOTA | 1730 | CD2 | | 218 | 18.862 | 22.464 | 65.903 | 1.00 40.08 | AAAA |
| | 1731 | C | LEU | 218 | 20.700 | 22.459 | 63.554 | 1.00 19.46 | AAAA |
| MOTA | 1732 | ŏ | LEU | 218 | 21.467 | 23.425 | 63.615- | 1.00 16.70 | AAAA |
| MOTA | | | ASN | 219 | 19.590 | 22.441 | 62.824 | 1.00 15.43 | AAAA |
| MOTA | 1733 | N | ASN | 219 | 19.143 | 23.609 | 62.072 | 1.00 14.05 | AAAA |
| MOTA | 1734 | CA | | 219 | 18.634 | 23.232 | 60.665 | 1.00 15.92 | AAAA |
| MOTA | 1735 | CB | ASN | | 19.732 | 22.738 | 59.750 | 1.00 22.73 | AAAA |
| MOTA | 1736 | CG | ASN | 219 | | 23.232 | 59.802 | 1.00 17.90 | AAAA |
| ATOM | 1737 | OD1 | | 219 | 20.861 | | 58.868 | 1.00 16.62 | AAAA |
| MOTA | 1738 | ND2 | | 219 | 19.398 | 21.789 | | 1.00 21.98 | AAAA |
| ATOM | 1739 | С | ASN | 219 | 17.990 | 24.256 | 62.821 | 1.00 21.38 | AAAA |
| MOTA | 1740 | 0 | ASN | 219 | 17.075 | 23.569 | 63.262 | | AAAA |
| ATOM | 1741 | N | ILE | 220 | 18.025 | 25.580 | 62.952 | 1.00 16.82 | |
| ATOM | 1742 | CA | ILE | 220 | 16.951 | 26.298 | 63.640 | 1.00 13.22 | AAAA |
| ATOM | 1743 | CB | ILE | 220 | 17.522 | 27.115 | 64.823 | 1.00 15.70 | AAAA |
| ATOM | 1744 | | ILE | 220 | 16.411 | 27.912 | 65.479 | 1.00 15.18 | AAAA |
| MOTA | 1745 | | ILE | 220 | 18.246 | 26.193 | 65.823 | 1.00 19.11 | AAAA |
| | 1746 | | ILE | 220 | 17.350 | 25.259 | 66.632 | 1.00 22.75 | AAAA |
| ATOM - | 1747 | C | ILE | 220 | 16.363 | 27.246 | 62.573 | 1.00 18.80 | AAAA |
| MOTA | 1748 | õ | ILE | 220 | 16.810 | 28.386 | 62.419 | 1.00 15.52 | AAAA |
| ATOM | | | PRO | 221 | 15.341 | 26.790 | 61.826 | 1.00 16.72 | AAAA |
| MOTA | 1749 | N | PRO | 221 . | 14.612 | 25.518 | 61.906 | 1.00 18.83 | AAAA |
| MOTA | 1750 | CD | PRO | 221 | 14.739 | 27.628 | 60.785 | 1.00 19.83 | AAAA |
| MOTA | 1751 | CA | | 221 | 13.930 | 26.615 | 59.948 | 1.00 20.76 | AAAA |
| MOTA | 1752 | CB | PRO | 221 | 14.409 | 25.241 | 60.462 | 1.00 28.73 | AAAA |
| MOTA | 1753 | CG | PRO | | 13.849 | 28.664 | 61.444 | 1.00 21.26 | AAAA |
| MOTA | 1754 | С | PRO | 221 | 13.061 | 28.318 | 62.314 | 1.00 22.45 | AAAA |
| MOTA | 1755 | 0 | PRO | 221 | | 29.926 | 61.028 | 1.00 19.70 | AAAA |
| ATOM | 1756 | N | LEU | 222 | 13.977 | | 61.612 | 1.00 21.62 | AAAA |
| ATOM | 1757 | CA | LEU | 222 | 13.209 | 31.018 | 62.319 | 1.00 16.46 | AAAA |
| ATOM | 1758 | CB | LEU | 222 | 14.163 | 31.972 | | 1.00 18.65 | AAAA |
| MOTA | 1759 | CG | LEU | 222 | 14.868 | 31.232 | 63.466 | 1.00 21.32 | AAAA |
| ATOM | 1760 | | LEU | 222 | 16.026 | 32.072 | 64.014 | | AAAA |
| ATOM | 1761 | CD2 | LEU | 222 | 13.857 | 30.925 | 64.555 | 1.00 19.98 | AAAA |
| ATOM | 1762 | С | LEU | 222 | 12.350 | 31.763 | 60.590 | 1.00 19.68 | AAAA |
| ATOM | 1763 | 0 | LEU | 222 | 12.687 | 31.830 | 59.412 | 1.00 18.07 | |
| ATOM | 1764 | N | PRO | 223 | 11.220 | 32.329 | 61.042 | 1.00 19.37 | AAAA |
| | 1765 | CD | PRO | 223 | 10.723 | 32.249 | 62.431 | 1.00 17.38 | AAAA |
| MOTA | 1766 | CA | PRO | 223 | 10.264 | 33.065 | 60.203 | 1.00 19.59 | AAAA |
| MOTA | 1767 | CB | PRO | 223 | 9.006 | 33.083 | 61.074 | 1.00 20.08 | AAAA |
| MOTA | 1101 | | PRO | 223 | 9.608 | 33.304 | 62.441 | 1.00 21.96 | AAAA |
| MOTA | 1768 | CG | PRO | 223 | 10.606 | 34.458 | 59.723 | 1.00 23.15 | AAAA |
| MOTA | 1769 | C | | 223 | 11.525 | 35.101 | 60.214 | 1.00 15.81 | AAAA |
| ATOM | 1770 | 0 | PRO | | 9.830 | 34.912 | 58.745 | 1.00 16.41 | AAAA |
| MOTA | 1771 | Ŋ | LYS | 224 | | 36.254 | 58.200 | 1.00 16.11 | AAAA |
| MOTA | 1772 | CA | LYS | 224 | 9.975 | | 57.039 | 1.00 20.34 | AAAA |
| MOTA | 1773 | CB | LYS | 224 | 9.002 | 36.446 | | 1.00 19.33 | AAAA |
| MOTA | 1774 | CG | LYS | 224 | 9.163 | 35.441 | 55.900 | 1.00 25.49 | AAAA |
| ATOM | 1775 | CD | LYS | 224 | 8.109 | 35.687 | 54.807 | 1.00 24.14 | AAAA |
| MOTA | 1776 | CE | LYS | 224 | 8.209 | 34.624 | 53.704 | 1.00 24.14 | AAAA |
| | 1777 | NZ | LYS | 224 | 7.207 | 34.843 | 52.618 | 1.00 34.08 | |
| ATOM | 1778 | c | LYS | 224 | 9.638 | 37.289 | 59.284 | 1.00 15.77 | AAAA |
| MOTA | | Ö | LYS | 224 | 8.819 | 37.032 | 60.186 | 1.00 21.07 | AAAA |
| ATOM | 1779 | N | GLY | 225 | 10.239 | 38.469 | 59.171 | 1.00 20.77 | AAAA |
| ATOM | 1780 | | GLY | 225 | 9.974 | 39.527 | 60.129 | 1.00 20.30 | AAAA |
| MOTA. | 1781 | CA | GLY | | 10.556 | 39.286 | | 1.00 20.63 | AAAA |
| ACOM C | 1782 | С | يري | | | | | | _ |

| ATOM | 1783 | 0 | GLY | 225 | 10.128 | 39.912 | 62.468 | 1.00 20.66 | AAAA |
|--------|------|--------------|-------|-------|--------|--------|----------|--------------|-------|
| MOTA | 1784 | N | LEU | 7 226 | 11.540 | 38.395 | 61.606 | 1.00 20.37 | AAAA |
| | | | | | | | | | |
| MOTA | 1785 | | | | 12.154 | | | 1.00 18.71 | AAAA |
| ATOM | 1786 | CB | LEU | 226 | 13.354 | 37.145 | 62.670 | 1.00 13.63 | AAAA |
| ATOM | 1787 | CG | LEU | 226 | 13.836 | 36.443 | 63.939 | 1.00 18.44 | AAAA |
| | | | | | | | | | |
| ATOM - | 1788 | | 1 LEU | | 12.834 | 35.329 | 64.243 | 1,00 18.09 | AAAA |
| MOTA | 1789 | CD: | 2 LEU | 226 | 15.232 | 35.844 | 63.741 | 1.00 17.96 | AAAA |
| MOTA | 1790 | С | LEU | 226 | 12.649 | 39.309 | 63.642 | 1.00 19.84 | ĀAAĀ |
| | | | | | | | | | |
| ATOM | 1791 | 0 | LEU | | 13.320 | 40.151 | 63.052 | 1.00 18.13 | AAAA |
| ATOM | 1792 | N | ASN | 227 | 12.336 | 39.421 | 64.932 | 1.00 23.30 | AAAA |
| ATOM | 1793 | CA | ASN | 227 | 12.815 | 40.571 | 65.692 | 1.00 20.88 | |
| | | | | | | | | | AAAA |
| MOTA | 1794 | CB | ASN | | 11.682 | 41.261 | 66.485 | 1.00 21.73 | AAAA |
| MOTA | 1795 | CG | ASN | 227 | 11.061 | 40.368 | 67.546 | - 1.00 20.47 | AAAA |
| MOTA | 1796 | op: | l ASN | 227 | 11.762 | 39.736 | 68.341 | 1.00 23.80 | AAAA |
| | | | | | 9.729 | 40.340 | | | |
| MOTA | 1797 | | 2 ASN | | | | 67.581 | 1.00 21.08 | AAAA |
| MOTA | 1798 | С | ASN | 227 | 13.950 | 40.152 | 66.612 | 1.00 25.24 | -AAAA |
| ATOM | 1799 | 0 | ASN | 227 | 14.282 | 38.965 | 66.702 | 1.00 18.54 | AAAA |
| | 1800 | N | ASP | | 14.547 | 41.124 | 67.296 | | |
| ATOM | | | | | | | | 1.00 19.41 | AAAA |
| ATOM | 1801 | CA | ASP | 228 | 15.682 | 40.844 | 68.169 | 1.00 22.15 | AAAA |
| ATOM | 1802 | CB | ASP | 228 | 16.208 | 42.141 | 68.802 | 1.00 16.82 | AAAA |
| ATOM | 1803 | CG | ASP | 228 | 16.852 | 43.060 | 67.796 | 1.00 30.68 | |
| | | | | | | | | | AAAA |
| ATOM | 1804 | | ASP | 228 | 17.182 | 42.576 | 66.690 | 1.00 23.87 | AAAA |
| ATOM | 1805 | OD2 | ASP | 228 | 17.053 | 44.256 | 68.123 | 1.00 25.02 | AAAA |
| ATOM | 1806 | С | ASP | 228 | 15.440 | 39.835 | 69.265 | 1.00 18.83 | AAAA |
| | | | | | | | | | |
| MOTA | 1807 | 0 | ASP | 228 | 16.298 | 39.002 | 69.536 | 1.00 16.28 | AAAA |
| MOTA | 1808 | N | ASN | 229 | 14.291 | 39.930 | 69.928 | 1.00 20.73 | AAAA |
| MOTA | 1809 | CA | ASN | 229 | 13.975 | 39.015 | 71.007 | 1.00 21.75 | AAAA |
| ATOM | 1810 | CB | ASN | 229 | 12.706 | 39.483 | 71.712 | 1.00 19.46 | |
| | - | | | | | | | | AAAA |
| MOTA | 1811 | CG | ASN | 229 | 12.943 | 40.738 | 72.516 | 1.00 27.14 | AAAA |
| ATOM | 1812 | OD1 | ASN | 229 | 13.588 | 40.691 | 73.556 | 1.00 33.03 | AAAA |
| ATOM | 1813 | MD2 | ASN | 229 | 12.464 | 41.874 | 72.019 | 1.00 21.35 | AAAA |
| | | | | | | | | | |
| ATOM | 1814 | С | ASN | 229 | 13.833 | 37.596 | 70.503 | 1.00 18.47 | AAAA |
| MOTA | 1815 | 0 | ASN | 229 | 14.284 | 36.644 | . 71.151 | 1.00 22.47 | AAAA |
| ATOM | 1816 | N | GLU | 230 | 13.252 | 37.454 | 69.319 | 1.00 17.79 | AAAA |
| ATOM | 1817 | CA | GLU | 230 | 13.081 | 36.125 | 68.748 | 1.00 21.18 | |
| | | | | | | | | | AAAA |
| ATOM | 1818 | CB | GLU | . 230 | 12.152 | 36.193 | 67.536 | 1.00 20.54 | AAAA |
| ATOM | 1819 | CG | GLU | 230 | 10.765 | 36.714 | 67.890 | 1.00 28.98 | AAAA |
| ATOM | 1820 | CD | GLU | 230 | 9.870 | 36.816 | 66.677 | 1.00 24.35 | AAAA |
| | 1821 | | | | | | | | |
| ATOM | | | GLU | 230 | 10.360 | 37.296 | 65.638 | 1.00 22.00 | AAAA |
| MOTA | 1822 | OE2 | GLU | 230 | 8.683 | 36.443 | 66.772 | 1.00 24.99 | AAAA |
| ATOM | 1823 | С | GLU | 230 | 14.422 | 35.507 | 68.361 | 1.00 16.89 | AAAA |
| ATOM | 1824 | 0 | GLU | 230 | 14.663 | 34.326 | 68.603 | 1.00 19.45 | AAAA |
| | | N | | | | | | | |
| ATOM | 1825 | | PHE | 231 | 15.305 | 36.305 | 67.772 | 1.00 15.68 | AAAA |
| ATOM | 1826 | CA | PHE | 231 | 16.616 | 35.788 | 67.389 | 1.00 15.78 | AAAA |
| ATOM | 1827 | CB | PHE | 231 | 17.420 | 36.863 | 66.649 | 1.00 13.22 | AAAA |
| MOTA | 1828 | CG | PHE | 231 | 18.719 | 36.361 | 66.069 | 1 90.20.63 | AAAA |
| | | | | | | | | | |
| MOTA | 1829 | | PHE | 231 | 18.723 | 35.445 | 65.016 | 1 00 18.42 | AAAA |
| MOTA | 1830 | CD2 | PHE | 231 | 19.936 | 36.804 | 66.568 | 1 70 21.10 | AAAA |
| ATOM | 1831 | CE1 | PHE | 231 | 19.918 | 34.983 | 64.471 | 1.00 17.67 | AAAA |
| ATOM | 1832 | | PHE | 231 | 21.144 | 36.346 | 66.029 | 1.00 28.29 | AAAA |
| | | | | | | | | | |
| MOTA | 1833 | CZ | PHE | 231 | 21.130 | 35.431 | 64.976 | 1.00 27.85 | AAAA |
| ATOM | 1834 | C | PHE | 231 | 17.385 | 35.332 | 68.636 | 1.00 18.54 | AAAA |
| MOTA | 1835 | 0 | PHE | 231 | 17.869 | 34.201 | 68.702 | 1.00 18.86 | AAAA |
| | | | | | | | | | |
| MOTA | 1836 | N | LEU | 232 | 17.495 | 36.204 | 69.636 | 1.00 19.07 | AAAA |
| ATOM | 1837 | CA | LEU | 232 | 18.239 | 35.850 | 70.848 | 1.00 17.39 | AAAA |
| ATOM | 1838 | CB | LEU | 232 | 18.415 | 37.078 | 71.737 | 1.00 24.53 | AAAA |
| | | | | | | | | 1.00 16.64 | AAAA |
| ATOM | 1839 | CG | LEU | 232 | 19.214 | 38.202 | 71.061 | | |
| ATOM | 1840 | CD1 | LEU | 232 | 19.134 | 39.449 | 71.934 | 1.00 26.70 | AAAA |
| MOTA | 1841 | CD2 | LEU | 232 | 20.659 | 37.806 | 70.810 | 1.00 18.77 | AAAA |
| | 1842 | c | LEU | 232 | 17.607 | 34.707 | 71.628 | 1.00 19.82 | AAAA |
| ATOM | | | | | | | • | | |
| ATOM | 1843 | 0 | LEU | 232 | 18.309 | 33.904 | 72.217 | 1.00 21.80 | AAAA |
| ATOM | 1844 | N | PHE | 233 | 16.281 | 34.640 | 71.648 | 1.00 17.18 | AAAA |
| ATOM | 1845 | CA | PHE | 233 | 15.587 | 33.537 | 72.309 | 1.00 23.34 | AAAA |
| | | | | | | | | 1.00 19.17 | |
| MOTA | 1846 | CB | PHE | 233 | 14.074 | 33.663 | 72:095 | | AAAA |
| ATOM | 1847 | CG | PHE | 233 | 13.289 | 32.447 | 72.523 | 1.00 21.40 | AAAA |
| ATOM | 1848 | CD1 | PHE | 233 | 12.863 | 32.302 | 73.841 | 1.00 29.62 | AAAA |
| | | - | | | | | • | | |

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| ATOM | 1849 | CD2 | PHE | 233 | 12.942 | 31.473 | 71.596 | 1.00 19.92 | AAAA |
|--------------|--------------|----------|------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 1850 | | PHE | 233 | 12.088 | 31.206 | 74.229 | 1.00 29.35 | AAAA |
| ATOM | 1851 | | PHE | 233 | 12.168 | 30.363 | 71.966 | 1.00 25.37 | AAAA |
| ATOM | 1852 | CZ | PHE | 233 | 11.737 | 30.231 | 73.283 | 1.00 30.28 | AAAA |
| ATOM | 1853 | С | PHE | 233 | 16.041 | 32.234 | 71.660 | 1.00 23.12 | AAAA |
| ATOM | 1854 | 0 | PHE | 233 | 16.433 | 31.273 | 72.332 | 1.00 18.35 | AAAA |
| MOTA | 1855 | N | ALA | 234 | 15.961 | 32.208 | 70.332 | 1.00 17.26 | AAAA |
| ATOM | 1856 | CA | ALA | 234 | 16.332 | 31.026 | 69.562 | 1.00 17.67 | AAAA |
| ATOM | 1857 | CB | ALA | 234 | 16.085 | 31.297 | 68.046 | 1.00 19.08 | AAAA |
| ATOM | 1858 | С | ALA | 234 | 17.786 | 30.641 | 69.800 | 1.00 16.31 | AAAA |
| MOTA | 1859 | 0 | ALA | 234 | 18.127 | 29.461 | 69.926 | 1.00 16.75 | AAAA |
| ATOM | 1860 | N | LEU | 235 | 18.646 | 31.643 | 69.846 | 1.00 16.73 | AAAA |
| ATOM | 1861 | CA | LEU | 235 | 20.074 | 31.411 | 70.051 | 1.00 19.14 | AAAA . |
| MOTA | 1862 | CB | LEU | 235 | 20.823 | 32.742 | 69.956 | 1.00 21.72 1.00 36.73 | AAAA |
| MOTA | 1863 | CG | LEU | 235 | 22.226 | 32.790 | 69.345 70.105 | 1.00 30.73 | AAAA AAAA |
| MOTA | 1864 | | LEU | 235 | 23.026 | 33.844 31.426 | 69.393 | 1.00 22.96 | AAAA |
| MOTA | 1865 | | LEU | 235 | 22.917 20.354 | 30.776 | 71.421 | 1.00 18.71 | AAAA |
| ATOM | 1866 | C | LEU | 235 | 21.028 | 29.747 | 71.522 | 1.00 18.59 | AAAA |
| MOTA | 1867 | 0 | LEU | 235 | 19.831 | 31.390 | 72.479 | 1.00 25.43 | AAAA |
| MOTA | 1868 | N | GLU | 236 236 | 20.046 | 30.883 | 73.839 | 1.00 19.75 | AAAA |
| ATOM | 1869 | CA CB | GLU GLU | 236 | 19.335 | 31.777 | 74.860 | 1.00 23.18 | AAAA |
| MOTA | 1870 | CG | GLU | 236 | 19.725 | 33.229 | 74.777 | 1.00 38.53 | AAAA |
| MOTA | 1871 1872 | CD | GLU | 236 | 18:857 | 34.119 | 75.648 | 1.00 42.42 | AAAA |
| MOTA MOTA | 1873 | | GLU | 236 | 17.617 | 34.171 | 75.428 | 1.00 45.43 | AAAA |
| ATOM | 1874 | OE2 | GLU | 236 | 19.425 | 34.768 | 76.548 | 1.00 48.76 | AAAA |
| ATOM | 1875 | C | GLU | 236 | 19.541 | 29.452 | 74.011 | 1.00 25.85 | AAAA |
| ATOM | 1876 | 0 | GLU | 236 | 20.222 | 28.603 | 74.597 | 1.00 21.36 | AAAA |
| ATOM | 1877 | Ŋ | LYS | 237 | 18.343 | 29.193 | 73.501 | 1.00 23.16 | AAAA |
| ATOM | 1878 | CA | LYS | 237 | 17.752 | 27.871 | 73.610 | 1.00 17.06 | AAAA |
| ATOM | 1879 | CB | LYS | 237 | 16.282 | 27.943 | 73.193 | 1.00 26.98 | AAAA |
| MOTA | 1880 | CG | LYS | 237 | 15.483 | 26.711 | 73.519 | 1.00 52.00 1.00 56.40 | AAAA AAAA |
| MOTA | 1881 | CD | LYS | 237 | 14.078 | 27.110 | 73.932 75.183 | 1.00 52.03 | AAAA |
| MOTA | 1882 | CE | LYS | 237 | 14.131 | 27.979 28.421 | 75.163 | 1.00 55.53 | AAAA |
| MOTA | 1883 | NZ | LYS | 237 | 12.782 18.502 | 26.827 | 72.785 | 1.00 18.46 | AAAA |
| MOTA | 1884 | C | LYS | 237 237 | 18.691 | 25.692 | 73.231 | 1.00 21.20 | AAAA |
| ATOM | 1885 | и | LYS SER | 238 | 18.932 | 27.187 | 71.578 | 1.00 21.28 | AAAA |
| MOTA | 1886 1887 | CA | SER | 238 | 19.649 | 26.208 | 70.776 | 1.00 16.47 | AAAA |
| ATOM | 1888 | CB | SER | 238 | 19.745 | 26.666 | 69.307 | 1.00 19.75 | AAAA |
| ATOM ATOM | 1889 | OG | SER | 238 | 20.475 | 27.858 | 69.160 | 1.00 22.52 | AAAA |
| MOTA | 1890 | C | SER | 238 | 21.039 | 25.923 | 71.361 | 1.00 18.79 | AAAA |
| ATOM | 1891 | 0 | SER | 238 | 21.521 | 24.788 | 71.312 | 1.00 20.60 | AAAA |
| MOTA | 1892 | N | LEU | 239 | 21.690 | 26.937 | 71.925 | 1.00 22.95 | AAAA |
| ATOM | 1893 | CA | LEU | 239 | 23.004 | 26.701 | 72.513 | 1.00 20.98 | AAAA |
| MOTA | 1894 | CB. | LEU | 239 | 23.652 | 28.008 | 72.986 | 1.00 18.39 | AAAA AAAA |
| MOTA | 1895 | CG | LEU | 239 | 23.985 | 29.072 | 71.933 | 1.00 20.02 1.00 27.02 | AAAA |
| ATOM | 1896 | | LEU | 239 | 24.538 | 30.311 | 72.636 70.933 | 1.00 27.02 | AAAA |
| MOTA | 1897 | CD2 | | 239 | 25.010 | 28.556 | 73.680 | 1.00 25.16 | AAAA |
| MOTA | 1898 | c | LEU | 239 | 22.882 | 25.735 24.929 | 73.920 | 1.00 20.70 | AAAA |
| ATOM | 1899 | 0 | LEU | 239 | 23.780 21.768 | 25.800 | 74.398 | 1.00 24.93 | AAAA |
| MOTA | 1900 | N | GLU | 240 | 21.700 | 24.912 | 75.536 | 1.00 25.72 | AAAA |
| MOTA | 1901 | CA | GLU GLU | 240 240 | 20.331 | 25.356 | 76.337 | 1.00 29.10 | AAAA |
| ATOM | 1902 | CB CG | GLU | 240 | 20.042 | 24.531 | 77.581 | 1.00 49.56 | AAAA |
| ATOM | 1903 1904 | CD | GLU | 240 | 19.053 | 25.212 | 78.515 | 1.00 63.15 | AAAA |
| ATOM | 1905 | OE1 | | 240 | 17.935 | 25.550 | 78.067 | 1.00 69.26 | AAAA |
| ATOM | 1905 | OE2 | | 240 | 19.400 | 25.410 | 79.703 | 1.00 66.68 | AAAA |
| ATOM | 1907 | C | GLU | 240 | 21.440 | 23.469 | 75.046 | 1.00 23.44 | AAAA |
| ATOM ATOM | 1908 | õ | GLU | 240 | 21.951 | 22.535 | 75.674 | 1.00 23.10 | AAAA |
| MOTA | 1909 | N | ILE | 241 | 20.771 | 23.294 | 73.913 | 1.00 19.52 | AAAA |
| ATOM | 1910 | CA | ILE | 241 | 20.598 | 21.978 | 73.321 | 1.00 24.06 | AAAA |
| ATOM | 1911 | CB | ILE | 241 | 19.705 | 22.039 | 72.052 | 1.00 23.80 | AAAA |
| ATOM | 1912 | CG2 | ILE | 241 | 19.718 | 20.678 | 71.323 | 1.00 24.94 | AAAA |
| ATOM | 1913 | CG1 | ILE | 241 | 18.281 | 22.433 | 72.439 | 1.00 28.60 | AAAA |
| ATOM | 1914 | CD1 | ILE | 241 | 17.336 | 22.600 | 71.257 | 1.00 27.04 | AAAA |

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| ATOM | 191 | | ILE | | 21.95 | 7 21.404 | 72.941 | | AAAA |
|--------------|----------------|---------|------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| MOTA | 191 | | IL | | 22.24 | | | | AAAA |
| ATOM ATOM | 191° 1918 | | VAI VAI | | 22.79: 24.11 | | | | AAAA |
| ATOM | 191 | | | | 24.85 | | | | AAAA |
| MOTA | 1920 | | 1 VAL | | 26.27 | | | | AAAA |
| ATOM | 192 | | 2 VAL | | 24.09 | | | | AAAA AAAA |
| MOTA | 1922 | 2 C | VAL | 242 | 24.962 | | | | AAAA |
| ATOM | 1923 | | VAL | | 25.566 | 20.384 | 73.235 | | AAAA |
| ATOM | 1924 | | LYS | | 24.989 | | | | AAAA |
| MOTA MOTA | 1925 1926 | | | | 25.775 | | | | AAAA |
| ATOM | 1927 | | | | 25.599 26.386 | | | | AAAA |
| ATOM | 1928 | | | | 26.022 | | | 1.00 43.21 1.00 53.10 | AAAA |
| ATOM | 1929 | | | 243 | 26.407 | | | | AAAA AAAA |
| MOTA | 1930 | | LYS | 243 | 26.045 | | | 1.00 59.15 | AAAA |
| MOTA | 1931 | | LYS | 243 | 25.433 | | | 1.00 30.38 | AAAA |
| MOTA | 1932 | | LYS | 243 | 26.321 | | | 1.00 35.44 | AAAA |
| ATOM ATOM | 1933 1934 | | GLU | 244 244 | 24.161 | | 76.076 | 1.00 28.12 | AAAA |
| ATOM | 1935 | | GLU | 244 | 23.798 22.288 | | 76.798 77.048 | 1.00 37.54 | AAAA |
| ATOM | 1936 | | GLU | 244 | 21.735 | | 77.816 | 1.00 35.34 1.00 55.88 | AAAA AAAA |
| ATOM | 1937 | CD | GLU | 244 | 20.281 | | 78.230 | 1.00 57.89 | AAAA |
| ATOM | 1938 | | l GLU | 244 | 19.673 | 21.246 | 78.738 | 1.00 60.60 | AAAA |
| ATOM | 1939 | | GLU | 244 | 19.753 | 19.152 | 78.062 | 1.00 57.73 | AAAA |
| MOTA MOTA | 1940 1941 | c o | GLU GLU | 244 244 | 24.231 24.294 | 18.034 | 76.102 | 1.00 38.17 | AAAA |
| ATOM | 1942 | Ŋ | VAL | 245 | 24.541 | 16.978 18.124 | 76.727 74.817 | 1.00 38.46 1.00 30.29 | AAAA |
| MOTA | 1943 | CA | VAL | 245 | 24.933 | 16.958 | 74.042 | 1.00 30.23 | AAAA AAAA |
| ATOM | 1944 | CB | VAL | 245 | 23.984 | 16.778 | 72.833 | 1.00 46.68 | AAAA |
| MOTA | 1945 | | VAL | 245 | 24.462 | 15.641 | 71.942 | 1.00 53.09 | AAAA |
| MOTA | 1946 1947 | | VAL | 245 | 22.581 | 16.488 | 73.327 | 1.00 54.19 | AAAA |
| ATOM ATOM | 1947 | 0 | VAL VAL | 245 245 | 26.364 26.915 | 16.982 15.939 | 73.508 | 1.00 34.90 | AAAA |
| MOTA | 1949 | N | PHE | 246 | 26.980 | 18.156 | 73.164 73.465 | 1.00 34.73 1.00 29.22 | AAAA |
| ATOM | 1950 | CA | PHE | 246 | 28.324 | 18.256 | 72.897 | 1.00 29.17 | AAAA AAAA |
| ATOM | 1951 | CB | PHE | 246 | 28.178 | 18.800 | 71.464 | 1.00 30.42 | AAAA |
| MOTA | 1952 | CG | PHE | 246 | 29.384 | 18.588 | 70.585 | 1.00 25.62 | AAAA |
| ATOM ATOM | 1953 . 1954 | | PHE PHE | 246 246 | 29.695 30.167 | 17.326 | 70.097 | 1.00 28.89 | AAAA |
| ATOM | 1955 | | PHE | 246 | 30.771 | 19.668 17.138 | 70.196 69.222 | 1.00 25.17 1.00 23.43 | AAAA |
| ATOM | 1956 | | PHE | 246 | 31.248 | 19.495 | 69.322 | 1.00 22.40 | AAAA AAAA |
| MOTA | 1957 | CZ | PHE | 246 | 31.549 | 18.236 | 68.835 | 1.00 19.88 | AAAA |
| ATOM | 1958 | C | PHE | 246 | 29.233 | 19.176 | 73.712 | 1.00 23.38 | AAAA |
| MOTA | 1959 1960 | O | PHE | 246 | 28.867 | 20.312 | 74.002 | 1.00 29.15 | AAAA |
| ATOM ATOM | 1961 | N CA | GLU | 247 247 | 30.410 31.395 | 18.682 19.481 | 74.094 74.841 | 1.00 29.73 1.00 28.10 | AAAA |
| ATOM | 1962 | CB | GLU | 247 | 31.912 | 18.726 | 76.074 | 1.00 28.10 | AAAA AAAA |
| MOTA | 1963 | CG | GLU | 247 | 30.972 | 18.707 | 77.286 | 1.00 60.78 | AAAA |
| ATOM | 1964 | CD | GLU | 247 | 29.700 | 17.892 | 77.077 | 1.00 70.07 | AAAA |
| MOTA | 1965 | OE1 | | 247 | 28.913 | 18.220 | 76.165 | 1.00 79.95 | AAAA |
| MOTA MOTA | 1966 1967 | C C | GLU GLU | 247 | 29.481 | 16.920 | 77.835 | 1.00 76.80 | AAAA |
| ATOM | 1968 | ō | GLU | 247 | 32.554 33.490 | 19.741 18.946 | 73.876 73.778 | 1.00 28.90 1.00 23.67 | AAAA |
| ATOM | 1969 | N | PRO | 248 | 32.531 | 20.891 | 73.778 | 1.00 25.02 | AAAA AAAA |
| MOTA | 1970 | CD | PRO | 248 | 31.574 | 22.003 | 73.310 | 1.00 27.23 | AAAA |
| ATOM | 1971 | CA | PRO | 248 | 33.566 | 21.249 | 72.209 | 1.00 28.06 | AAAA |
| ATOM | 1972 | CB | PRO | 248 | 33.050 | 22.575 | 71.639 | 1.00 28.11 | AAAA |
| ATOM | 1973 1974 | CG | PRO | 248 | 31.551 | 22.512 | 71.897 | 1.00 34.57 | AAAA |
| ATOM ATOM | 1975 | С 0 | PRO PRO | 248 248 | 34.968 35.132 | 21.416 21.897 | 72.770 73.887 | 1.00 23.87 1.00 24.05 | AAAA |
| ATOM | 1976 | | GLU | 249 | 35.965 | 21.013 | 71.983 | 1.00 24.33 | AAAA AAAA |
| ATOM | 1977 | | GLU | 249 | 37.366 | 21.195 | 72.355 | 1.00 25.98 | AAAA |
| ATOM · | 1978 | CB | GLU | 249 | 38.275 | 20.166 | 71.679 | 1.00 22.07 | AAAA |
| ATOM | 1979 | | GLU | 249 | 38.046 | 18.726 | 72.116 | 1.00 33.40 | AAAA |
| ATOM | 1980 | CD | GLU | 249 | 39.005 | 17.767 | 71.445 | 1.00 29.15 | AAAA |
| • | | | | | | | | | _ |

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Figure 16-31

| ATOM | 1981 | OFI | GLU | 249 | 39.071 | 17.770 | 70.199 | 1.00 27.62 | AAAA |
|------|-------|-----|-----|------|----------|--------|--------|------------|------|
| | | | | | | 17.004 | 72.161 | 1.00 26.19 | |
| MOTA | 1982 | OE2 | _ | 249 | 39.694 | | | | AAAA |
| MOTA | 1983 | С | GLU | 249 | 37.692 | 22.561 | 71.786 | 1.00 26.04 | AAAA |
| MOTA | 1984 | 0 | GLU | 249 | 38.582 | 23.271 | 72.262 | 1.00 26.39 | AAAA |
| ATOM | 1985 | N | VAL | 250 | 36.953 | 22.921 | 70.744 | 1.00 23.83 | AAAA |
| MOTA | 1986 | CA | VAL | 250 | 37.151 | 24.197 | 70.086 | 1.00 19.67 | AAAA |
| | 1987 | CB | VAL | 250 | 38.438 | 24.178 | 69.210 | 1.00 20.88 | AAAA |
| MOTA | | | - | | | | | | |
| MOTA | 1988 | | VAL | 250 | 38.348 | 23.117 | 68.128 | 1.00 18.18 | AAAA |
| ATOM | 1989 | CG2 | VAL | .250 | 38.647 | 25.530 | 68.591 | 1.00 16.71 | AAAA |
| ATOM | 1990 | С | VAL | 250 | 35.946 | 24.483 | 69.207 | 1.00 20.78 | AAAA |
| ATOM | 1991 | 0 | VAL | 250 | . 35.299 | 23.556 | 68.746 | 1.00 19.60 | AAAA |
| ATOM | 1992 | N | TYR | 251 | 35.633 | 25.757 | 69.000 | 1.00 18.75 | AAAA |
| | 1993 | | | 251 | 34.497 | 26.109 | 68.153 | 1.00 22.44 | ÀAAA |
| MOTA | | CA | TYR | | | 26.437 | 69.022 | 1.00 16.57 | |
| ATOM | 1994 | CB | TYR | 251 | 33.261 | | | | AAAA |
| ATOM | 1995 | CG | TYR | 251 | 33.207 | 27.856 | 69.575 | 1.00 22.36 | AAAA |
| ATOM | 1996 | CD1 | TYR | 251 | 32.654 | 28.896 | 68.823 | 1.00 18.12 | AAAA |
| MOTA | 1997 | CE1 | TYR | 251 | 32.612 | 30.185 | 69.308 | 1.00 20.40 | AAAA |
| ATOM | 1998 | CD2 | | 251 | 33.715 | 28.160 | 70.842 | 1.00 20.04 | AAAA |
| | 1999 | CE2 | | 251 | 33.676 | 29.475 | 71.349 | 1.00 16.60 | AAAA |
| MOTA | | | | | | 30.473 | 70.573 | 1.00 14.68 | AAAA |
| MOTA | 2000 | CZ | TYR | 251 | 33.128 | | | | |
| MOTA | 2001 | он | TYR | 251 | 33.100 | 31.780 | 71.011 | 1.00 21.79 | AAAA |
| MOTA | 2002 | С | TYR | 251 | 34.811 | 27.294 | 67.236 | 1.00 20.28 | AAAA |
| MOTA | 2003 | 0 | TYR | 251 | 35.695 | 28.107 | 67.525 | 1.00 19.91 | AAAA |
| ATOM | 2004 | N | LEU | 252 | 34.097 | 27.360 | 66.109 | 1.00 17.90 | AAAA |
| ATOM | 2005 | CA | LEU | 252 | 34.216 | 28.466 | 65.161 | 1.00 18.58 | AAAA |
| | 2005 | CB | LEU | 252 | 34.679 | 28.001 | 63.767 | 1.00 17.55 | AAAA |
| ATOM | | | | | | 27.290 | 63.718 | 1.00 23.36 | AAAA |
| MOTA | 2007 | CG | LEU | 252 | 36.028 | | | | |
| ATOM | 2008 | | LEU | 252 | 35.819 | 25.820 | 64.017 | 1.00 27.78 | AAAA |
| ATOM | 2009 | CD2 | LEU | 252 | 36.631 | 27.440 | 62.331 | 1.00 27.29 | AAAA |
| ATOM | 2010 | С | LEU | 252 | 32.816 | 29.049 | 65.052 | 1.00 15.49 | AAAA |
| ATOM | 2011 | 0 | LEU | 252 | 31.819 | 28.320 | 65.120 | 1.00 18.82 | AAAA |
| ATOM | 2012 | N | LEU | 253 | 32.756 | 30.360 | 64.891 | 1.00 16.80 | AAAA |
| ATOM | 2013 | CA | LEU | 253 | 31.498 | 31.105 | 64.817 | 1.00 17.50 | AAAA |
| | 2014 | CB | LEU | 253 | 31.379 | 31.987 | 66.073 | 1.00 15.49 | AAAA |
| ATOM | | | | | 30.326 | 33.085 | 66.165 | 1.00 17.75 | AAAA |
| MOTA | 2015 | CG | LEU | 253 | | | | | AAAA |
| ATOM | 2016 | | LEU | 253 | 28.946 | 32.438 | 66.172 | 1.00 20.85 | |
| ATOM | 2017 | CD2 | LEU | 253 | 30.536 | 33.897 | 67.464 | 1.00 19.05 | AAAA |
| ATOM | 2018 | С | LEU | 253 | 31.516 | 31.985 | 63.580 | 1.00 20.22 | AAAA |
| MOTA | 2019 | 0 | LEU | 253 | 32.474 | 32.727 | 63.371 | 1.00 18.14 | AAAA |
| ATOM | 2020 | N | GLN | 254 | 30.466 | 31.913 | 62.765 | 1.00 16.50 | AAAA |
| ATOM | 2021 | CA | GLN | 254 | 30.411 | 32.730 | 61.556 | 1.00 16.48 | AAAA |
| | 2022 | СВ | GLN | 254 | 30.085 | 31.863 | 60.312 | 1.00 25.58 | AAAA |
| ATOM | | | | 254 | 28.647 | 31.798 | 59.871 | 1.00 36.40 | AAAA |
| MOTA | 2023 | CG | GLN | | | | 58.701 | 1.00 33.18 | AAAA |
| ATOM | 2024 | CD | GLN | 254 | 28.337 | 32.728 | | | |
| MOTA | 2025 | | GLN | 254 | 28.744 | 32.487 | 57.546 | 1.00 21.05 | AAAA |
| ATOM | 2026 | NE2 | GLN | 254 | 27.613 | 33.799 | 58.992 | 1.00 22.85 | AAAA |
| ATOM | 2027 | C | GLN | 254 | 29.384 | 33.816 | 61.832 | 1.00 16.12 | AAAA |
| ATOM | 20285 | 0 | GLN | 254 | 28.282 | 33.577 | 62.364 | 1.00 13.97 | AAAA |
| ATOM | 2029 | N | LEU | 255 | 29.768 | 35.032 | 61.468 | 1.00 14.42 | AAAA |
| | 2030 | CA | LEU | 255 | 28.988 | 36.215 | 61.763 | 1.00 17.99 | AAAA |
| MOTA | | | | | | | 62.719 | 1.00 20.68 | AAAA |
| MOTA | 2031 | CB | LEU | 255 | | 37.070 | | | |
| MOTA | 2032 | CG | LEU | 255 | 30.240 | 36.283 | 63.964 | 1.00 22.90 | AAAA |
| MOTA | 2033 | CD1 | LEU | 255 | 31.446 | 36.906 | 64.635 | 1.00 29.36 | AAAA |
| ATOM | 2034 | CD2 | LEU | 255 | 29.042 | 36.214 | 64.900 | 1.00 14.80 | AAAA |
| ATOM | 2035 | С | LEU | 255 | 28.541 | 37.060 | 60.594 | 1.00 19.32 | AAAA |
| | 2036 | ŏ | LEU | 255 | 28.838 | 38.260 | 60.561 | 1.00 21.23 | AAAA |
| ATOM | | | GLY | 256 | 27.827 | 36.467 | 59.639 | 1.00 17.21 | AAAA |
| ATOM | 2037 | N | | | | | 58.516 | 1.00 15.64 | AAAA |
| MOTA | 2038 | CA | GLY | 256 | 27.347 | 37.259 | | | |
| MOTA | 2039 | С | GLY | 256 | 26.413 | 38.348 | 59.028 | 1.00 17.31 | AAAA |
| ATOM | 2040 | 0 | GLY | 256 | 25.717 | 38.150 | 60.027 | 1.00 15.62 | AAAA |
| ATOM | 2041 | N | THR | 257 | 26.389 | 39.494 | 58.348 | 1.00 19.72 | AAAA |
| ATOM | 2042 | CA | THR | 257 | 25.536 | 40.598 | 58.776 | 1.00 19.88 | AAAA |
| | | CB | THR | 257 | 26.242 | 41.973 | 58.589 | 1.00 14.02 | AAAA |
| MOTA | 2043 | OG1 | | 257 | 26.538 | 42.187 | 57.206 | 1.00 17.58 | AAAA |
| MOTA | 2044 | | | | | | 59.392 | 1.00 19.67 | AAAA |
| MOTA | 2045 | CG2 | | 257 | 27.543 | 42.009 | | | |
| MOTA | 2046 | С | THR | 257 | 24.199 | 40.634 | 58.053 | 1.00 20.58 | AAAA |

| ATOM | | | | | 23.40 | 3 41.545 | 5 58.266 | 1.00 14.59 | AAAA |
|--------------|--------------|----------|--------------|------------|------------------|------------------|------------------|----------------------------|--------------|
| MOTA | | | _ | | 23.92 | | | 1.00 16.56 | AAAA |
| MOTA MOTA | | | | | 22.65 | | | | AAAA |
| ATOM | 205 | | | | 22.60 23.03 | | | | AAAA |
| ATOM | | | D1 ASI | | 23.22 | | | | AAAA |
| MOTA | 205 | | D2 ASE | | 23.18 | | | | AAAA AAAA |
| MOTA | 205 | - | | | 21.39 | | | | ÄAAA |
| ATOM | 205 | _ | | | 20.300 | | | | AAAA |
| ATOM ATOM | 205 205 | | | | 21.510 22.614 | | | | AAAA |
| ATOM | 205 | | | | 20.281 | | | | AAAA |
| ATOM | 205 | | | | 20.710 | | | 1.00 21.24 - 1.00 21.18 | AAAA AAAA |
| MOTA | 206 | | PRO | 259 | 22.174 | | 60.846 | | AAAA |
| ATOM | 206 | | PRO | | 19.705 | | | 1.00 20.88 | AAAA |
| MOTA MOTA | 206: 206: | | PRO | | 18.572 | | | | -AAAA |
| ATOM | 206 | | LEU LEU | | 20.473 20.023 | | | 1.00 18.75 | AAAA |
| ATOM | 206 | | | | 21.202 | | | 1.00 22.16 1.00 20.35 | AAAA |
| MOTA | 2066 | | LEU | | 22.403 | | | 1.00 21.82 | AAAA AAAA |
| MOTA | 206 | | 1 LEU | 260 | 23.604 | 44.486 | | 1.00 18.57 | AAAA |
| ATOM | 2068 | | 2 LEU | 260 | 22.032 | | | 1.00 19.18 | AAAA |
| MOTA MOTA | 2069 2070 | | LEU LEU | 260 260 | 18.876 18.742 | | | 1.00 24.16 | AAAA |
| ATOM | 2071 | | LEU | 261 | 18.049 | | 57.826 59.634 | 1.00 21.69 1.00 19.54 | AAAA |
| ATOM | 2072 | | | 261 | 16.903 | | 58.965 | 1.00 17.34 | AAAA AAAA |
| ATOM | 2073 | | | 261 | 16.285 | 45.967 | 59.892 | 1.00 19.96 | AAAA |
| ATOM ATOM | 2074 2075 | | LEU 1 LEU | - | 15.204 | 46.879 | 59.300 | 1.00 29.99 | AAAA |
| ATOM | 2076 | | 2 LEU | 261 261 | 14.080 14.682 | | 58.732 | 1.00 33.66 | AAAA |
| ATOM | 2077 | | LEU | 261 | 17.262 | 47.819 45.550 | 60.376 57.620 | 1.00 44.71 1.00 18.11 | AAAA |
| MOTA | 2078 | | LEU | 261 | 16.539 | 45.386 | 56.634 | 1.00 19.02 | AAAA AAAA |
| ATOM | 2079 | | GLU | 262 | 18.391 | 46.249 | 57.566 | 1.00 22.68 | AAAA |
| ATOM ATOM | 2080 2081 | CA CB | GLU | 262 | | 46.921 | 56.338 | 1.00 18.46 | AAAA |
| ATOM | 2082 | CG | GLU | 262 262 | 19.875 19.365 | 47.965 49.136 | 56.641 | 1.00 22.01 | AAAA |
| ATOM | 2083 | CD | GLU | 262 | 19.434 | 48.902 | 57.443 58.927 | 1.00 22.94 1.00 23.11 | AAAA AAAA |
| ATOM | 2084 | | GLU | 262 | 19.668 | 47.748 | 59.357 | 1.00 24.58 | AAAA |
| ATOM | 2085 | | GLU | 262 | 19.238 | 49.883 | 59.667 | 1.00 27.06 | AAAA |
| ATOM ATOM | 2086 2087 | С 0 | GLU GLU | 262 262 | 19.281 19.446 | 46.034 | 55.197 | 1.00 25.65 | AAAA |
| ATOM | 2088 | N | ASP | 263 | 19.501 | 46.510 44.750 | 54.070 55.467 | 1.00 25.49 1.00 22.45 | AAAA |
| ATOM | 2089 | CA | ASP | 263 | 19.959 | 43.851 | 54.418 | 1.00 22.45 | AAAA AAAA |
| ATOM | 2090 | CB | ASP | 263 | 20.981 | 42.859 | 54.988 | 1.00 18.99 | AAAA |
| ATOM | 2091 | CG | ASP | 263 | 21.706 | 42.081 | 53.907 | 1.00 22.21 | AAAA |
| ATOM ATOM | 2092 2093 | | ASP ASP | 263 263 | 22.876 21.112 | 41.730 | 54.139 | 1.00 23.19 | AAAA |
| ATOM | 2094 | C | ASP | 263 | 18.733 | 41.809 43.165 | 52.838 53.837 | 1.00 25.02 1.00 22.32 | AAAA - |
| ATOM | 2095 | ō | ASP | 263 | 18.012 | 42.419 | 54.519 | 1.00 22.32 | AAAA AAAA |
| ATOM | 2096 | N | TYR | 264 | 18.500 | 43.447 | 52.564 | 1.00 25.21 | AAAA |
| ATOM | 2097 | CA | TYR | 264 | 17.339 | 42.936 | 51.865 | 1.00 29.92 | AAAA |
| MOTA MOTA | 2098 2099 | CB CG | TYR | 264 | 17.077 | 43.776 | 50.596 | 1.00 38.48 | AAAA |
| ATOM | 2100 | | TYR TYR | 264 264 | 17.910 17.677 | 43.431 42.249 | 49.379 48.660 | 1.00 54.09 1.00 69.38 | AAAA |
| MOTA | 2101 | | TYR | 264 | 18.420 | 41.930 | 47.526 | 1.00 69.38 | AAAA AAAA |
| ATOM | 2102 | | TYR | 264 | 18.915 | 44.286 | 48.928 | 1.00 66.09 | AAAA |
| MOTA | 2103 | | TYR | 264 | 19.670 | 43.975 | 47.788 | 1.00 74.50 | AAAA |
| ATOM | 2104 | CZ | TYR | 264 | 19.415 | 42.794 | 47.094 | 1.00 72.57 | AAAA |
| MOTA MOTA | 2105 2106 | OH C | TYR TYR | 264 264 | 20.154 17.445 | 42.472 41.461 | 45.975 | 1.00 71.96 | AAAA |
| ATOM | 2107 | 0 | TYR | 264 | 16.448 | 40.839 | 51.532 51.190 | 1.00 29.55 | AAAA AAAA |
| MOTA | 2108 | | LEU | 265 | | 40.891 | 51.629 | 1.00 30.11 | AAAA AAAA |
| MOTA | 2109 | | L:EU | 265 | 18.753 | 39.476 | 51.337 | 1.00 25.36 | AAAA |
| MOTA | 2110 | | LEU | 265 | 20.186 | 39.089 | 50.969 | 1.00 29.81 | AAAA |
| ATOM MOTE | 2111 2112 | | LEU | 265 265 | 20.509 | 39.510 | 49.531 | 1.00 34.43 | AAAA |
| MOTA | كللت | CD1 | الطب | 265 | 21.847 | 38.930 | 49.100 | 1.00 44.38 | AAAA |

| * *0 | | AAAA |
|--|---|-------------|
| | 19 422 38.990 48.603 1.00 46.72 | AAAA |
| CD2 UEU 265 | 19.422 30,595 52.447 1.00 22.33 | AAAA |
| ATOM 2113 CD2 1110 265 | 18.209 30011. =2 348 1.00 23.30 | AAAA |
| 2114 C 1110 | 18.477 3 1 1 2 508 1.00 17.50 | AAAA |
| ATOM OTHER LEU ZON | 17.677 39.194 54.569 1.00 19.69 | - |
| ATOM SER 200 | 17 055 38.390 35 045 1 00 20.73 | AAAA |
| ATOM SER 266 | 17 012 38.314 33.100 1 nn 22.81 | AAAA |
| ATOM 411' CTD 266 | 17.55 20 442 56.684 1.55 25 | AAAA |
| ATOM ZIIO II CER 266 | 20 048 54.930 1.00 22 66 | AAAA |
| ATOM ZIII OF OFF 266 | 13.100 40 265 54.840 1.00 10 40 | AAAA |
| ATOM 2120 C 350 266 | 13.37 20 229 55.402 1.00 72.64 | AAAA |
| 2121 U 3111 207 | 14 799 JUIL - art 1 00 ZUIU | AAAA |
| -move 2122 N Bib | 13 52/ 30···· rib 1 NO 20·30 | AAAA |
| Alon old Ch LYS 201 | 12 397 37.70 | AAAA |
| ATOM 222 CB LYS 26/ | 12 269 37.330 33.47 | |
| ATTENDED CG DIE | 12 095 38.023 35 882 1 00 38.49 | AAAA |
| 7 TY 100 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 | 12.095 38.540 51.772 1.00 33.11 | AAAA |
| ATOM 2120 00 367 | 77 70 703 50.331 77 00 63 | AAAA |
| ATOM 2127 TVC 267 | 11.71 20 QR7 57.300 1.01 25 30 | AAAA |
| ATOM 2128 NZ 257 | 10. 10. 10. 10. 10. 10. 10. 10. 10. 10. | AAAA |
| атом 2129 С Б15 267 | 10 584 55.22 - 016 1 00 10.30 | AAAA |
| 2130 0 220 | 14.814 38.937 50 345 1.00 18.50 | AAAA |
| 2131 N PHE 200 | 15 034 39.182 22 1 00 20.91 | AAAA |
| ATOM CA PHE 200 | 16 328 38.510 5.007 1 00 16.96 | |
| ATOM 2133 CB PHE 268 | 16 252 37.000 33.415 1 00 16.61 | AAAA |
| ATOM 2133 CC PHE 268 | 10,12, 26 300 60,413 1,62 40 43 | AAAA |
| ATOM 2134 cm pur 268 | 26 303 59.004 203 | AAAA |
| ATOM 2135 CD1 PUF 268 | 13.01 34 QU4 60.381 1.01 18 45 | AAAA |
| NOM 2136 CD2 112 268 | 17.331 34 900 59.849 1.00 17.33 | AAAA |
| ATOM 2137 CE1 212 268 | 15.02/ 54.55 60 296 1.00 10.02 | AAAA |
| 2138 CEZ PRE 269 | 16.144 33 50 510 1.00 10.33 | AAAA |
| 2139 CZ PHE 200 | 15.1/9 40.00 60.20 | AAAA |
| 2140 C PRE 200 | 15 733 41.3/1 30.613 3 00 21.04 | AAAA |
| AIOI | 14 679 41.238 00.550 1 00 22.89 | AAAA |
| AION OLAS N ASN 200 | 14 763 42.6/3 3.640 1 00 20.55 | |
| ATOM 2143 CA ASN 269 | 12 365 43.298 60.940 1 00 26.13 | AAAA |
| 70M 4143 259 | 12 551 43.071. 59.000 1.00 29.17 | AAAA |
| arom 4144 - arm 269 | 12.060 43.192 58.371 1.00 28.26 | AAAA |
| 300M 4145 55 260 | 10 767 59.000 10 00 | AAAA |
| ATOM 2146 UDI ADN 269 | 12 967 62.139 1.00 21 95 | AAAA |
| ATTOM 2147 ND2 1011 269 | 15.493 43 683 63.019 1.00 21.71 | AAAA |
| ATOM 2148 C 750 269 | 14.984 43.435 62.298 1.00 17.53 | AAAA |
| NEOM 2149 0 270 | 16.695 42.40 63 521 1.00 10.51 | AAAA |
| 2150 N LEU 270 | 17.441 42.042 63 712 1.00 18.93 | AAAA |
| 2151 CA LEU 270 | 19 441 41.507 55 1 1 00 20.54 | AAAA |
| ATES CH LEU ZI | 17 945 40.000 00.000 1 00 14.19 | AAAA |
| ATOM 2153 CG LEU 270 | 10 070 39.1/4 03.165 1 00 19.05 | |
| ATOM 2155 CD1 LEU 270 | 16 679 39.833 03.503 1 00 22.83 | AAAA |
| | 18 203 43.971 63.363 1 00 18.25 | AAAA. |
| AUON 222 1 270 | 44 643 62.300 | AAAA |
| 740M 4130 270 | 44 318 64./33 4.0 20 | |
| ATOM 2157 0 220 271 | 10.1 46 E18 92.001 1. 10 13 | AAAA |
| ATOM 2158 N 3200 271 | 19.414 46 150 66.409 1.00 10.70 | AAAA |
| NTOM 2159 CA 321 | 18.985 40.227 67.512 1.00 22.20 | AAAA |
| NOM 2160 CB 3500 271 | 19.34/ 45.073 65.224 1.00 19.00 | AAAA |
| 2161 OG SER 271 | 20.875 | |
| 2162 C SER 272 | 21.122 43.833 65 020 1.00 16.1 | , |
| 24.53 O SER 2'- | 24 028 45.334 00 100 20.7 | 0 |
| Alon. | 22 270 45.693 37.4 | 9 |
| ATOM 2165 CA ASN 272 | 24 176 46.903 64.603 1 00 54.5 | 3 |
| ATOM 2103 01 272 | 47 378 63.403 | |
| λτOM 2100 02 277 | 2 40 A5A 63.133 TO 5 | 3 |
| ATOM 2167 CG HOW 272 | 46 594 62.575 | 1 3 |
| ATOM 2168 UD1 ACM 27 | 23.576 45.343 66.580 1.00 10. | AAAA 8 |
| ATOM 2169 ND2 1007 27 | 2 23.586 44.625 66.854 1.00 10. | |
| 2170 C ASN 27 | 24.545 44.625 67.500 1.00 19. | , , , , , , |
| 2171 O ASN 27 | 2 22 22 22 22 22 22 22 22 22 22 22 22 2 | 12 |
| ATOM 2112 N VAL 27 | 22 053 45.698 00 26. | 91 |
| ALON CA VAL | 22 345 46./62 23 1 00 39. | 69 |
| ATOM 21/3 CB VAL 27 | 22 440 46.444 15 22 1 00 34. | 13 |
| ATOM 21/4 CC1 VAL 27 | | 00 |
| TOM 2175 CG1 VIII. 27 | | 89 AAAA |
| 3TOM 21/6 CGD 2 | 12 22.636 44.22 70 217 1.00 10 | • |
| 3TOM 2177 C 377 2 | 73 23.249 43.708 70.22 | |
| ATOM 2178 O VAL 2 | ·. · | |
| ATOM | | |
| altharm | | |
| | | |

52/263 Figure 16-34

| MOTA | 217 | | ALA | A 274 | 21.601 | 43.747 | 68.713 | 1.00 21.79 | AAAA |
|--------------|-------|------|------------|------------|------------------|------------------|------------------|--------------------------|------|
| MOTA | 218 | 0 C. | A ALA | A 274 | 21.207 | 42.383 | 69.035 | | AAAA |
| ATOM | 218 | 1 C | B ALA | A 274 | 19.806 | | | | AAAA |
| ATOM | 218 | 2 C | ALA | 274 | 22.259 | | | | AAAA |
| ATOM | 218 | 3 0 | ALA | 274 | 22.569 | | | | AAAA |
| ATOM | 218 | 4 N | PHE | 275 | 22.798 | | | | AAAA |
| MOTA | 218 | 5 C | A PHE | 275 | 23.828 | | | | AAAA |
| ATOM | 218 | 6 CI | B PHE | | 24.220 | | | | |
| MOTA | 218 | 7 C | | | 25.363 | | | | AAAA |
| ATOM | 218 | | ol PHE | | 25.209 | | | | AAAA |
| ATOM | 2189 | | 2 PHE | | 26.590 | | | | AAAA |
| ATOM | 219 | | 1 PHE | | 26.266 | | | | AAAA |
| MOTA | 219 | | 2 PHE | | 27.654 | | | | AAAA |
| ATOM | 2192 | | | | 27.489 | | | | AAAA |
| ATOM | 2193 | | PHE | | | | | 1.00 24.63 1.00 25.06 | AAAA |
| ATOM | 2194 | | PHE | | 25.619 | | | | AAAA |
| ATOM | 2195 | | LEU | | 25.366 | | | 1.00 19.71 | AAAA |
| ATOM | 2196 | | | | 26.482 | | | 1.00 17.49 | AAAA |
| ATOM | 2197 | | | | 26.736 | | | 1.00 24.23 | AAAA |
| ATOM | 2198 | | | | 28.001 | | | 1.00 20.44 | AAAA |
| ATOM | 2199 | | 1 LEU | | 27.948 | 43.967 | | 1.00 39.65 | AAAA |
| ATOM | 2200 | | 2 LEU | 276 | | 45.447 | | 1.00 29.65 | AAAA |
| ATOM | 2201 | | LEU | 276 | 28.102 | 43.143 | 71.460 | 1.00 32.41 | AAAA |
| ATOM | 2202 | | LEU | 276 | 26.180 | 41.278 | 70.262 | 1.00 18.88 | AAAA |
| ATOM | 2202 | | LYS | 277 | 27.045 | 40.529 | 70.727 | 1.00 17.99 | AAAA |
| ATOM | 2204 | | | 277 | 24.968 | 41.374 | 70.805 | 1.00 19.67 | AAAA |
| ATOM | 2205 | | LYS | 277 | 24.644 | 40.552 | 71.964 | 1.00 21.33 | AAAA |
| ATOM | 2206 | | LYS | 277 | 23.265 | 40.888 | 72.532 | 1.00 23.84 | AAAA |
| ATOM | 2207 | | LYS | 277 | 23.247 | 42.126 | 73.366 | 1.00 40.87 | AAAA |
| MOTA | 2208 | CE | LYS | 277 | 22.069 | 42.086 | 74.325 | 1.00 54.73 | AAAA |
| ATOM | 2209 | NZ | LYS | 277 | 22.172 | 40.884 | 75.254 | 1.00 58.85 | AAAA |
| ATOM | 2210 | C | LYS | 277 | 21.051 | 40.844 | 76.228 | 1.00 55.34 | AAAA |
| ATOM | 2211 | Ö | LYS | 277 | 24.695 | 39.068 | 71.660 | 1.00 22.12 | AAAA |
| ATOM | 2212 | N | ALA | 278 | 25.074 24.311 | 38.264 | 72.513 | 1.00 22.19 | AAAA |
| ATOM | .2213 | CA | ALA | 278 | 24.311 | 38.700 37.291 | 70.441 | 1.00 20.23 | AAAA |
| ATOM | 2214 | CB | ALA | 278 | 23.798 | 37.154 | 70.039 | 1.00 17.06 | AAAA |
| ATOM | 2215 | c | ALA | 278 | 25.760 | 36.767 | 68.589 | 1.00 19.27 | AAAA |
| ATOM | 2216 | ō | ALA | 278 | 26.035 | 35.676 | 70.127 | 1.00 16:94 | AAAA |
| ATOM | 2217 | N | PHE | 279 | 26.679 | 37.564 | 70.648 | 1.00 14.93 | AAAA |
| ATOM | 2218 | CA | PHE | 279 | 28.099 | 37.231 | 69.606 | 1.00 18.88 | AAAA |
| ATOM | 2219 | CB | PHE | 279 | 28.880 | 38.392 | 69.626 | 1.00 21.01 | AAAA |
| ATOM | 2220 | CG | PHE | 279 | 30.370 | 38.264 | 68.998 69.120 | 1.00 16.79 | AAAA |
| ATOM | 2221 | | PHE | 279 | 31.062 | 37.272 | | 1.00 20.23 | AAAA |
| ATOM | 2222 | CD2 | | 279 | 31.088 | 39.159 | 68.423 | 1.00 21.61 | AAAA |
| ATOM | 2223 | | PHE | 279 | 32.461 | 37.185 | 69.905 68.509 | 1.00 23.24 | AAAA |
| ATOM | 2224 | CE2 | | 279 | 32.480 | 39.081 | 69.995 | 1.00 30.98 | AAAA |
| ATOM | 2225 | CZ | PHE | 279 | 33.169 | 38.095 | 69.295 | 1.00 24.82 | AAAA |
| ATOM | 2226 | c | PHE | 279 | 28.576 | 36.995 | 71.067 | 1.00 30.27 | AAAA |
| ATOM | 2227 | ŏ | PHE | 279 | 29.275 | 36.016 | 71.362 | 1.00 25.48 | AAAA |
| ATOM | 2228 | N | ASN | 280 | 28.194 | 37.898 | 71.962 | 1.00 16.30 | AAAA |
| ATOM | 2229 | CA | ASN | 280 | 28.599 | 37.777 | 73.352 | 1.00 22.30 | AAAA |
| ATOM | 2230 | CB | ASN | 280 | 28.391 | 39.109 | 74.080 | 1.00 24.49 1.00 27.17 | AAAA |
| ATOM | 2231 | CG | ASN | 280 | 29.344 | 40.183 | 73.578 | | AAAA |
| ATOM | 2232 | | ASN | 280 | 30.503 | 39.897 | 73.273 | 1.00 20.88 | AAAA |
| ATOM | 2233 | ND2 | | 280 | 28.875 | | 73.522 | 1.00 22.95 | AAAA |
| ATOM | 2234 | c | ASN | 280 | 27.928 | 41.421 36.636 | | 1.00 27.85 | AAAA |
| | 2235 | ō | | | | | 74.095 | 1.00 23.01 | AAAA |
| MOTA MOTA | 2236 | N | ASN ILE | 280 281 | 28.510 26.711 | 36.062 | 75.016 | 1.00 21.91 | AAAA |
| ATOM | 2237 | CA | ILE | 281 | | 36.300 | 73.689 | 1.00 18.74 | AAAA |
| | 2238 | | | 281 | 26.005 | 35.179 | 74.294 | 1.00 18.37 | AAAA |
| MOTA | | CB | ILE | 281 | 24.566 | 35.067 | 73.758 | 1.00 19.31 | AAAA |
| MOTA | 2239 | CG2 | ILE | 281 | 23.977 | 33.725 | 74.135 | 1.00 28.87 | AAAA |
| ATOM | 2240 | CG1 | ILE | 281 | 23.710 | 36.206 | 74.308 | 1.00 23.51 | AAAA |
| MOTA | 2241 | CD1 | ILE | 281 | 22.279 | 36.193 | 73.776 | 1.00 26.47 | AAAA |
| MOTA | 2242 | C | ILE | 281 | 26.743 | 33.876 | 73.965 | 1.00 18.54 | AAAA |
| MOTA | 2243 | 0 | ILE | 281 | 26.830 | 32.973 | 74.801 | 1.00 19.69 | AAAA |
| MOTA | 2244 | N | VAL | 282 | 27.258 | 33.765 | 72.744 | 1.00 17.72 | AAAA |
| | | | | | | | | | |

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| ATOM | 2245 | CA | VAL | 282 | 27.976 | 32,553 | 72.352 | 1.00 14 | . 89 | AAAA |
|--------|--------|---------------|------|-----|--------|--------|----------|---------|-------|------|
| | | | | | | | 70.852 | 1.00 18 | 50 | |
| ATOM | 2246 | CB | VAL | 282 | 28.359 | 32.565 | | | | AAAA |
| ATOM | 2247 | CG1 | VAL | 282 | 29.342 | 31.440 | 70.567 | 1.00 20 |).73 | AAAA |
| | | | | | 27.105 | 32.363 | 69.994 | 1.00 17 | 7 / 0 | AAAA |
| ATOM | 2248 | CGZ | VAL | 282 | | | | | | |
| ATOM | 2249 | С | VAL | 282 | 29.241 | 32.433 | 73.198 | 1.00 21 | 79 | AAAA |
| | | 0 | VAL | 282 | 29.568 | 31.360 | 73.715 | 1.00 25 | C R O | AAAA |
| ATOM | 2250 | Ų | | | | | | | | |
| MOTA | 2251 | N | ARG | 283 | 29.935 | 33.549 | 73.361 | 1.00 19 | 7.14 | AAAA |
| | 2252. | CA | ARG | 283 | 31.161 | 33.548 | 74.150 | 1.00 23 | 51 | AAAA |
| ATOM | | | | | | | | | | |
| ATOM | 2253 | CB | ARG | 283 | 31.851 | 34.898 | 74.023 | 1.00 20 |).64 | AAAA |
| ATOM | 2254 | CG | ARG | 283 | 32.338 | 35.200 | 72.607 | 1.00 19 | 1.65 | AAAA |
| | | | | | | | | | | |
| MOTA | 2255 | $^{\rm CD}$ | ARG | 283 | 32.754 | 36.645 | 72.474 | 1.00 25 | | AAAA |
| ATOM | 2256 | NE | ARG | 283 | 33.970 | 36.944 | 73.215 | 1.00 36 | 5.05 | AAAA |
| | | | | | 34.277 | 38.147 | 73.681 | 1.00 34 | | AAAA |
| ATOM | 2257 | \mathbf{cz} | ARG | 283 | | | | | | |
| ATOM | 2258 | NH1 | ARG | 283 | 33.448 | 39.169 | 73.488 | 1.00 35 | .23 | AAAA |
| | 2259 | MILES | ARG | 283 | 35.419 | 38.332 | 74.326 | 1.00 29 | 1.30 | AAAA |
| ATOM | | | | | | | | | | |
| MOTA | 2260 | С | ARG | 283 | 30.911 | 33.219 | 75.622 | 1.00 25 | .44 | AAAA |
| ATOM | 2261 | 0 | ARG | 283 | 31.754 | 32.600 | 76.272 | 1.00 23 | . 12 | AAAA |
| | | | | | | | | | | |
| ATOM | 2262 | N | GLU | 284 | 29.765 | 33.632 | 76.151 | 1.00 26 | | AAAA |
| ATOM | 2263 | CA | GLU | 284 | 29.462 | 33.338 | 77.553 | 1.00 31 | 77 | AAAA |
| | | | GLU | 284 | 28.243 | 34.115 | 78.033 | 1.00 30 | 0.6 | AAAA |
| ATOM | 2264 | CB | | | | | | | | |
| ATOM | 2265 | CG | GLU | 284 | 28.399 | 35.605 | 77.957 | 1.00 50 | 1.56 | AAAA |
| | 2266 | CD | GLU | 284 | 27.137 | 36.320 | 78.365 | 1.00 63 | .75 | AAAA |
| ATOM | | | | | | | | | | |
| MOTA | 2267 | OET | GLU | 284 | 26.085 | 36.067 | 77.738 | 1.00 68 | | AAAA |
| ATOM | 2268 | OE2 | GLU | 284 | 27.198 | 37.133 | 79.309 | 1.00 72 | 2.01 | AAAA |
| | | | | | 29.181 | 31.862 | 77.733 | 1.00 31 | | AAAA |
| MOTA | 2269 | С | GLU | 284 | | | | | | |
| ATOM | 2270 | 0 | GLU | 284 | 29.410 | 31.310 | 78.803 | 1.00 33 | 1.08 | AAAA |
| | 2271 | N | VAL | 285 | 28.673 | 31.221 | 76.686 | 1.00 23 | 1.37 | AAAA |
| ATOM | | | | | | | | | | |
| ATOM | 2272 | CA | VAL | 285 | 28.354 | 29.807 | 76.774 | 1.00 23 | | AAAA |
| ATOM | 2273 | CB | VAL | 285 | 27.221 | 29.407 | 75.789 | 1.00 24 | 1.77 | AAAA |
| | | | | | 26.952 | 27.913 | 75.881 | 1.00 26 | : 0Ω | AAAA |
| MOTA | 2274 | | VAL | 285 | | | | | | |
| ATOM | 2275 | CG2 | VAL | 285 | 25.940 | 30.181 | 76.107 | 1.00 24 | 1.98 | AAAA |
| MOTA | 2276 | С | VAL | 285 | 29.567 | 28.942 | 76.479 | 1.00 31 | . 41 | AAAA |
| | | | | | | | | 1.00 25 | | AAAA |
| ATOM | 2277 - | 0 | VAL | 285 | 29.833 | 27.983 | 77.195 | | | |
| ATOM | 2278 | N | PHE | 286 | 30.316 | 29.276 | . 75.431 | 1.00 27 | 1.27 | AAAA |
| | | CA | PHE | 286 | 31.463 | 28.457 | 75.086 | 1.00 22 | Δ7 | AAAA |
| ATOM | 2279 | | | | | | | | | |
| ATOM | 2280 | CB | PHE | 286 | 31.289 | 27.904 | 73.667 | 1.00 22 | 2.26 | AAAA |
| ATOM | 2281 | CG | PHE | 286 | 30.168 | 26.918 | 73.536 | 1.00 25 | 5.71 | AAAA |
| | | | | | | | | 1.00 22 | | AAAA |
| ATOM | 2282 | CD1 | PHE | 286 | 28.971 | 27.274 | 72.917 | | | |
| ATOM | 2283 | CD2 | PHE | 286 | 30.294 | 25.631 | 74.069 | 1.00 24 | 1.49 | AAAA |
| | | CE1 | | 286 | 27.919 | 26.365 | 72.829 | 1.00 19 | . 85 | AAAA |
| ATOM . | 2284 | | | | | | | | | |
| ATOM | 2285 | CE2 | PHE | 286 | 29.246 | 24.714 | 73.987 | 1.00 27 | | AAAA |
| ATOM | 2286 | CZ | PHE | 286 | 28.056 | 25.081 | 73.367 | 1.00 24 | 1.59 | AAAA |
| | | | | | 32.854 | 29.059 | 75.225 | 1.00 21 | 53 | AAAA |
| MOTA | 2287 | С | PHE | 286 | | | | | | |
| MOTA | 2288 | 0 | PHE | 286 | 33.849 | 28.417 | 74.873 | 1.00 27 | 1.12 | AAAA |
| ATOM | 2289 | N | GLY | 287 | 32.937 | 30.272 | 75.754 | 1.00 23 | .76 | AAAA |
| | | | | | | | | | | |
| ATOM | 2290 | CA | GLY | 287 | 34.237 | 30.896 | 75 901 | 1.00 24 | | AAAA |
| ATOM | 2291 | С | GLY | 287 | 34.705 | 31.419 | 74.562 | 1.00 27 | 7.05 | AAAA |
| | | | | 287 | 33.888 | | .73.667 | 1.00 18 | | AAAA |
| MOTA | 2292 | 0 | GLY | | _ | | | | | |
| ATOM | 2293 | N | GLU | 288 | 36.017 | 31.576 | 74.414 | 1.00 23 | 3.21 | AAAA |
| | 2294 | CA | GLU | 288 | 36.583 | 32.085 | 73.170 | 1.00 24 | 1.87 | AAAA |
| MOTA | | | | | | | | | | AAAA |
| ATOM | 2295 | CB | GLU | 288 | 37.968 | 32.682 | 73.410 | 1.00 29 | | |
| ATOM | 2296 | CG | GLU | 288 | 37.984 | 33.933 | 74.291 | 1.00 42 | 2.63 | AAAA |
| | | | | 288 | 37.114 | 35.052 | 73.745 | 1.00 43 | 1 77 | AAAA |
| ATOM | 2297 | CD | GLU | | | | | | | |
| ATOM | 2298 | OE1 | GLU | 288 | 37.235 | 35.380 | 72.544 | 1.00 36 | | AAAA |
| | 2299 | | GLU | 288 | 36.317 | 35.617 | 74.521 | 1.00 51 | 56 | AAAA |
| ATOM | | | | | | | | 1.00 20 | ١ ٥٥ | AAAA |
| MOTA | 2300 | С | GLU | 288 | 36.693 | 31.028 | 72.072 | | | |
| ATOM | 2301 | 0 | GLU | 288 | 36.995 | 29.856 | 72.332 | 1.00 18 | 3.10 | AAAA |
| | | | | 289 | 36.447 | 31.468 | 70.843 | 1.00 26 | | AAAA |
| ATOM | 2302 | N | GLY | | | | | | | |
| ATOM | 2303 | CA | GLY | 289 | 36.517 | 30.588 | 69.692 | 1.00 20 | 7.71 | AAAA |
| | | | GLY | 289 | 37.126 | 31.318 | 68.510 | 1.00 18 | 3.56 | AAAA |
| ATOM | 2304 | С | | | | | | | | |
| ATOM | 2305 | 0 | GLY | 289 | 37.669 | 32.404 | 68.679 | 1.00 16 | | AAAA |
| | 2306 | N | VAL | 290 | 37.032 | 30.724 | 67.322 | 1.00 19 | 3.86 | AAAA |
| ATOM | | | | | | | 66.103 | 1.00 19 | 7.70 | AAAA |
| MOTA | 2307 | CA | VAL | 290 | 37.572 | 31.312 | | | | |
| ATOM | 2308 | CB | VAL | 290 | 38.150 | 30.192 | 65.184 | 1.00 19 | | AAAA |
| | | CG1 | | 290 | 38.667 | 30.769 | 63.853 | 1.00 15 | 5.54 | AAAA |
| ATOM | 2309 | | **** | | _ | | | 1.00 20 | | AAAA |
| ATOM | 2310 | CG2 | ٧AL | 290 | 39.296 | 29.483 | 65.920 | 1.00 20 | | WANT |

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| : | | | | | | | | | | | |
|------|-------|------|--------|-------|-------|-------------|--------|----------|-------|----------|-----------|
| ATOM | | | | | 36 | .408 | 32.04 | | 7 1.0 | 00 20.90 | AAAA |
| ATOM | | | VAI | L 290 | 35 | .351 | 31.43 | 9 65.19 | | 00 19.33 | AAAA |
| MOTA | 231 | .3 N | TY! | R 291 | 36 | .598 | 33.32 | | | 00 15.37 | |
| ATOM | 231 | 4 C | A TY | R 291 | | . 543 | 34.14 | | | | AAAA |
| MOTA | 231 | 5 C | B TY | | | .412 | 35.43 | | | 00 16.79 | AAAA |
| ATOM | | | G TY | | | .375 | | | 1.0 | 0 16.42 | AAAA |
| ATOM | | _ | D1 TYP | | | | 35.18 | | | 00 18.60 | AAAA |
| MOTA | | _ | - | | | .366 | 35.68 | | 9 1.0 | 00 21.77 | AAAA |
| | | | E1 TYF | | | . 368 | 35.38 | 5 69.030 | 1.0 | 0 22.55 | AAAA |
| ATOM | | | D2 TYF | | 34 | .388 | 34.37 | 4 67.361 | | 0 17.34 | AAAA |
| MOTA | | | E2 TYF | | 34 | .381 | 34.06 | 68.718 | 1.0 | 0 20.24 | AAAA |
| ATOM | 232 | 1 C | Z TYF | 291 | | . 367 | 34.568 | | | 0 25.85 | |
| ATOM | 232 | 2 0 | H TYR | 291 | | .338 | 34.246 | | | | AAAA |
| ATOM | 232 | | | | | 720 | 34.446 | | | 0 25.57 | , AAAA |
| ATOM | 2324 | | | | | | | | 1.0 | 0 14.97 | AAAA |
| ATOM | 232 | | | | | . 773 | 34.921 | | 1.0 | 0 15.21 | AAAA |
| | | | | | | . 660 | 34.189 | | 1.0 | 0 14.06 | AAAA |
| ATOM | 2326 | | | | | 674 | 34.392 | 60.824 | 1.0 | 0 15.03 | AAAA |
| ATOM | 2327 | | | | 34. | 461 | 33.046 | 60.108 | | 0 13.66 | AAAA |
| MOTA | 2328 | 3 C | G LEU | 292 | 35. | 342 | 31.856 | | | 0 19.04 | |
| MOTA | 2329 | CI | Ol LEU | 292 | 34. | 909 | 30.615 | | | 0 15.17 | AAAA |
| ATOM | 2330 |) CI | O2 LEU | | | 792 | 32.190 | 60.252 | | | AAAA |
| MOTA | 2331 | | LEU | 292 | | 564 | | | | 0 19.18 | AAAA |
| ATOM | 2332 | | LEU | 292 | | | 35.327 | | | 0 16.62 | AAAA |
| MOTA | 2333 | | | | | 57 5 | 35.488 | | | 0 14.76 | AAAA |
| | | | GLY | 293 | | 724 | 35.932 | | 1.0 | 0 18.62 | AAAA |
| ATOM | 2334 | | | 293 | | 696 | 36.816 | | 1.0 | 0 17.10 | AAAA |
| MOTA | 2335 | | GLY | 293 | .31. | 611 | 35.954 | 58.068 | | 0 23.44 | AAAA |
| ATOM | 2336 | | GLY | 293 | 31. | 407 | 34.798 | 58.459 | | 0 23.60 | AAAA |
| ATOM | 2337 | N | GLY | 294 | 30. | 915 | 36.501 | | | 0 24.96 | |
| MOTA | 2338 | CA | GLY | 294 | 29. | 871 | 35.738 | | | 0 27.07 | AAAA |
| ATOM | 2339 | С | .GLY | 294 | | 132 | 36.632 | 55.474 | | | AAAA |
| ATOM | 2340 | 0 | GLY | 294 | 29. | | 37.722 | | | 28.41 | AAAA |
| ATOM | 2341 | N | GLY. | 295 | 27. | | | 55.167 | | 25.66 | AAAA |
| ATOM | 2342 | CA | | 295 | | | 36.168 | | | 20.33 | AAAA |
| ATOM | 2343 | | | | 27. | | 36.936 | 54.085 | 1.00 | 20.14 | AAAA |
| | | C | GLY | 295 | 26. | | 38.244 | 54.730 | 1.00 | 25.34 | AAAA |
| ATOM | 2344 | .0 | GLY | 295 | 26. | | 38.317 | 55.942 | 1.00 | 28.89 | AAAA |
| ATOM | 2345 | N | GLY | 296 | 26. | 514 | 39.274 | 53.909 | | 28.52 | AAAA |
| ATOM | 2346 | CA | GLY | 296 | 26.2 | 230 | 40.598 | 54.367 | | 23.21 | AAAA |
| MOTA | 2347 | C | GLY | 296 | 26.3 | 314 | 41.342 | 53.059 | | 26.34 | AAAA |
| ATOM | 2348 | 0 | GLY | 296 | 27.3 | | 41.324 | 52.414 | | 26.05 | |
| ATOM | 2349 | N | TYR | 297 | 25.2 | | 42.008 | 52.662 | | 22.61 | AAAA |
| ATOM | 2350 | CA | TYR | 297 | 25.2 | | 42.644 | | | | AAAA |
| ATOM | 2351 | СВ | TYR | 297 | 24.2 | | | 51.360 | | 22.58 | AAAA |
| MOTA | 2352 | CG | TYR | 297 | | | 41.861 | 50.457 | | 23.68 | AAAA |
| ATOM | 2353 | | | | 24.5 | | 40.352 | 50.521 | | 25.14 | AAAA |
| | | | TYR | 297 | 23.9 | | 39.571 | 51.568 | 1.00 | 28.31 | AAAA |
| ATOM | 2354 | | TYR | 297 | 24.2 | | 38.196 | 51.662 | 1.00 | 24.18 | AAAA |
| ATOM | 2355 | | TYR | 297 | 25.3 | | 39.725 | 49.577 | 1.00 | 29.74 | AAAA |
| MOTA | 2: 56 | | TYR | 297 | 25.5 | 98 | 38.362 | 49.664 | | 27.09 | AAAA |
| ATOM | 257 | CZ | TYR | 297 | 25.0 | 85 | 37.606 | 50.696 | | 28.68 | AAAA |
| MOTA | 2538 | ОН | TYR | 297 | 25.4 | | 36.261 | 50.739 | | 28.17 | AAAA |
| ATOM | 2359 | С | TYR | 297 | 24.9 | | 44.138 | 51.320 | | 24.98 | |
| ATOM | 2360 | 0 | TYR | 297 | 24.8 | | 44.714 | 50.237 | | 26.51 | AAAA |
| ATOM | 2361 | N. | HIS | 298 | 24.7 | | 4.752 | 52.491 | | | AAAA |
| ATOM | 2362 | CA | HIS | 298 | 24.4 | | | | | 23.80 | AAAA |
| ATOM | 2363 | | HIS | | | | 6.188 | 52.591 | | 23.44 | AAAA |
| | | | | 298 | 23.3 | ' | 16.494 | 53.536 | | 23.37 | AAAA |
| ATOM | 2364 | CG | HIS | 298 | 22.9 | _ | 17.945 | 53.551 | 1.00 | 32.94 | AAAA |
| MOTA | 2365 | | HIS | 298 | 23.4 | _ | 18.983 | 54.232 | 1.00 | 24.31 | AAAA |
| ATOM | 2366 | | HIS | 298 | 22.0 | l1 4 | 8.487 | 52.707 | 1.00 | 38.29 | AAAA |
| ATOM | 2367 | CE1 | HIS | 298 | 21.9 | 78 4 | 9.797 | 52.868 | | 26.60 | AAAA |
| ATOM | 2368 | NE2 | HIS | 298 | 22.8 | | 0.125 | 53.788 | | 36.57 | |
| MOTA | 2369 | C | HIS | 298 | 25.7 | | 6.775 | | | | AAAA |
| ATOM | 2370 | ō | HIS | 298 | 26.1 | | | 53.184 | | 23.11 | AAAA |
| ATOM | 2371 | N | PRO | 298 | | | 6.439 | 54.306 | | 22.64 | AAAA |
| | | | | | 26.43 | | 7.673 | 52.445 | | 21.07 | AAAA |
| ATOM | 2372 | CD | PRO | 299 | 26.07 | | 8.207 | 51.117 | 1.00 | 27.42 | AAAA |
| ATOM | 2373 | CA | PRO | 299 | 27.67 | _ | 8.286 | 52,910 | | 26.62 | AAAA |
| | 2374 | CB | PRO | 299 | 28.04 | | 9.228 | 51.755 | | 28.95 | AAAA |
| ATOM | 2375 | CG | PRO | 299 | 26.67 | 8 4 | 9.600 | 51.196 | | 35.16 | AAAA |
| MOTA | 2376 | С | PRO | 299 | 27.64 | | 8.991 | 54.262 | | 25.75 | AAAA |
| | | _ | | | | • | | | 1.00 | | * = -5474 |

SUBSTITUTE SHEET (RULE 26)

55/263 Figure 16-37

| Figur | re 10-3/ | AAA |
|--|---------------------------------------|---|
| | EE 068 1.00 24.50 | AAAA |
| 2377 O PRO 299 2 | 18.565 40.769 54.504 1.00 24.40 | AAAA |
| ATOM 23/ TYR 300 | 26.602 50 478 55.766 1.00 22.34 | AAAA |
| ATOM 2376 CA TVR 300 | 51 442 55.754 1.50 20 44 | AAAA |
| ληΟΜ 43/3 ° 300 4 | E2 509 54./04 T. 07 03 | AAAA |
| ATOM 2300 CC TVR 300 | 266 52 634 53.74 1 20 20 66 | AAAA |
| DI TYK | 26 389 53.676 52.813 1.00 31.37 | AAAA |
| ATOM 2383 CE1 TYR 300 | 24 490 53.640 54.827 1 00 35.88 | AAAA |
| ATOM 2394 CD2 TYR 300 | 24 501 54.677 53.910 1 00 38.44 | AAAA |
| ATOM 2385 CE2 TYR 300 | 25.448 54.689 54.000 1 00 33.41 | AAAA |
| 2386 CZ TYR 300 | 25 417 55.700 22.80 | AAAA AAAA |
| ATOM 2387 OR 111 300 | 26.280 49.515 57.983 1.00 19.14 | AAAA |
| ATOM 2388 C 111 300 | 26.833 48 568 56.705 1.00 23.00 | AAAA |
| ATOM 2389 0 111 301 | 25.374 47 509 57.719 1.00 21.00 | AAAA |
| ATOM 2390 N ALA 301 | 25.009 47.597 57.198 1.00 19.32 | AAAA |
| ATOM 2394 Th NTN 301 | 23.032 46 762 58.098 1.00 | AAAA |
| ATOM 2332 - 27 A 301 | 26 507 46.570 59.274 1.00 23.19 | AAAA |
| ATOM 2393 O ALA 301 | 26 904 46.275 57.072 1.00 20.66 | AAAA |
| ATOM 2394 N LEU 302 | 28 090 45.463 57.234 1 00 23.31 | AAAA |
| ATOM 2396 CA LEU 302 | 28 602 45 057 55 637 1 00 36 66 | AAAA |
| ATOM 2207 CB LEU . 302 | 29.932 44.333 54.170 1.00 38.41 | AAAA AAAA |
| ATOM 2208 CG LEU 302 | 29 979 43.849 = 270 1 00 28.52 | AAAA |
| | 31.104 45.435 58 012 1.00 22.08 | AAAA |
| ATOM 2400 CD2 DD3 302 | 29.163 45 713 59.020 1.00 20.43 | AAAA |
| ATOM 2401 2 1EU 302 | 47 401 57.545 1.05 10 77 | AAAA |
| ATOM 2402 TA 303 | 20 567 48.173 58.197 1 00 21.69 | AAAA |
| ATOM 2403 CA ALA 303 | 30.816 49.460 57.432 1.00 19.19 | AAAA |
| ATOM 2405 CB ALA 303 | 30.324 48.485 50 489 1.00 22.51 | AAAA AAAA |
| amon 2406 C ALA 303 | 21 216 48.310 50.603 1 00 20.12 | AAAA |
| ATOM 2407 0 ADA 304 | 29.128 48.934 61.377 1.00 18.04 | AAAA |
| ATOM 2408 N ARG 304 | 28.872 50 334 61.511 1.00 21.34 | AAAA |
| ATOM 2409 CA 7110 304 | 21.22 51 401 60.792 2.00 60 | AAAA |
| ATOM 2410 CG ARG 304 | 26 259 52.259 61.206 1.00 45.73 | AAAA |
| ATOM 2412 CD ARG 304 | 25 090 51.398 61.110 1 00 39.82 | A AAA A AAA |
| ATOM 2413 NE ARG 304 | 23.965 51.549 62.677 1.00 28.40 | AAAA |
| 2414 CZ ARG | 23.813 52.330 61 647 1.00 41.// | AAAA |
| ATOM 2415 NAT ARG 304 | 22.991 30.073 62.280 1.00 21.03 | AAAA |
| ATOM 2416 NHZ ARC 304 | 20 213 48.087 63.397 1 00 19.93 | AAAA |
| ATOM 2417 C ARG 304 | 20 159 47.008 61.750 1.00 18.70 | AAAA |
| ATOM 2410 N ALA 305 | 28 002 45.809 62.613 1 00 18.26 | AAAA AAAA |
| 7420 CA ALA 305 | 26.998 44.830 62.915 1.00 16.46 | AAAA. |
| NTOM 2421 CB ALA 305 | 29.311 45.109 64.061 1.00 19.49 | AAAA |
| ATOM 2422 C ALA 305 | 29.504 44.009 61.905 1.00 4.00 | AAAA |
| ATOM 2423 TRP 306 | 30.132 44 268 62.183 1.00 10.06 | AAAA |
| ATOM 2424 mpp 306 | 20 151 43.865 60.902 1.00 21.34 | AAAA |
| ATOM 2425 CB TRP 306 | 31 632 42.564 60.333 1 00 16.55 | AAAA |
| ATOM 2427 CG TRP 306 | 31 852 42.058 59.019 1 00 19.37 | AAAA AAAA |
| 2428 CD2 TRP 300 | 31.243 40.783 57.878 1.00 17.80 | AAAA |
| 2429 CE2 TRP 300 | 32.507 43 610 60.995 1.00 15.05 | |
| ATOM 2430 CE3 TRP 306 ATOM 2431 CD1 TRP 306 | 30.919 40.535 60.170 1.00 13.95 | , |
| ATOM 2431 CD1 TRD 306 | 30.680 40.002 57.787 1.00 24.66 | ,~ |
| ATOM 2432 CZ2 TRP 306 | 32 534 41.781 56.723 1.00 17.04 | 1= |
| ATOM 2433 CZ3 TRP 306 | 31 917 40.513 56.831 1.00 20.20 | |
| ATOM 2435 CH2 TRP 306 | 32 289 45.168 63.010 1.00 21.2 | ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, |
| ATOM 2436 C TRP 306 | 33.159 44./26 62 911 1.00 18.6 | 0 |
| ATOM 2437 O TRP 306 | 32.061 46.491 63.722 1.00 16.8 | 8 |
| STOM 2438 N THR 307 | 32.843 47.412 63.312 1.00 22.0 | AAAA B |
| ATOM 2439 THR 307 | 32.579 40.000 62.051 1.00 21.7 | AAAA |
| ATOM . 2440 CB THR 307 | 126 49 857 64.330 | • |
| ATOM 2441 CG2 THR 307 | | |
| ATOM 2442 CG2 1111 | | |
| Allharm | A A A A A A A A A A A A A A A A A A A | |

| MOTA | 2443 | С | THE | 307 | 32.493 | 47.146 | 65.187 | 1.00 17.47 | AAAA |
|--------------|--------------|----------|------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 2444 | | THE | | 33.377 | 47.142 | 66.039 | | AAAA |
| ATOM | 2445 | | LEU | | 31.216 | 46.901 | 65.487 | 1.00 19.97 | AAAA |
| ATOM | 2446 | | | | 30.834 | | | | AAAA |
| ATOM | 2447 | | | | 29.318 | | | | AAAA |
| ATOM | 2448 | | | | 28.415 | | | | AAAA |
| ATOM | 2449 | | 1 LEU | | 26.937 | | | | AAAA |
| MOTA | 2450 | | 2 LEU | | 28.870 | | | | AAAA |
| ATOM ATOM | 2451 2452 | | LEU LEU | | 31.578 32.056 | | | | AAAA |
| ATOM | 2453 | | ILE | | 31.677 | | | 1.00 22.27 | AAAA |
| ATOM | 2454 | | ILE | | 32.377 | | | 1.00 22.54 1.00 17.09 | AAAA |
| ATOM | 2455 | | ILE | | 32.318 | | | 1.00 17.03 | AAAA AAAA |
| ATOM | 2456 | | 2 ILE | | 33.170 | | | 1.00 24.16 | AAAA |
| ATOM | 2457 | CG: | l ILE | 309 | 30.871 | | | 1.00 18.26 | AAAA |
| ATOM | 2458 | CD: | l, ILE | 309 | 30.205 | | | 1.00 26.57 | AAAA |
| MOTA | 2459 | С | ILE | 309 | 33.849 | 43.410 | 67.067 | 1.00 20.84 | AAAA |
| ATOM | 2460 | 0 | ILE | 309 | 34.426 | 42.905 | 68.031 | 1.00 25.20 | AAAA |
| ATOM | 2461 | N | TRP | 310 | 34.466 | 44.223 | 66.214 | 1.00 16.86 | AAAA |
| ATOM | 2462 | .CA | TRP | 310 | 35.888 | 44.517 | 66.411 | 1.00 17.86 | AAAA |
| ATOM | 2463 | CB | TRP | 310 | 36.439 | 45.319 | 65.235 | 1.00 14.83 | AAAA |
| MOTA MOTA | 2464 2465 | CG | TRP TRP | 310 310 | 37.879 38.967 | 45.648 | 65.397 | 1.00 16.63 | AAAA |
| ATOM | 2466 | | TRP | 310 | 40.131 | 44.718 45.478 | 65.560 65.799 | 1.00 18.62 | AAAA |
| ATOM | 2467 | CE3 | | 310 | 39.069 | 43.319 | 65.529 | 1.00 25.60 1.00 24.06 | AAAA AAAA |
| ATOM | 2468 | | TRP | 310 | 38.418 | 46.895 | 65.533 | 1.00 19.82 | AAAA |
| ATOM | 2469 | NE1 | TRP | 310 | 39.768 | 46.801 | 65.777 | 1.00 25.84 | AAAA |
| MOTA | 2470 | CZ2 | TRP | 310 | 41.383 | 44.887 | 66.006 | 1.00 26.14 | AAAA |
| MOTA | 2471 | CZ3 | | 310 | 40.308 | 42.730 | 65.735 | 1.00 24.89 | AAAA |
| MOTA | 2472 | | TRP | 310 | 41.452 | 43.515 | 65.971 | 1.00 24.96 | AAAA |
| MOTA | 2473 | C | TRP | 310 | 36.112 | 45.263 | 67.733 | 1.00 20.86 | AAAA |
| MOTA MOTA | 2474 2475 | O N | TRP CYS | 310 311 | 37.050 | 44.957 | 68.476 | 1.00 21.38 | AAAA |
| ATOM | 2476 | CA | CYS | 311 | 35.242 35.349 | 46.226 46.971 | 68.030 69.280 | 1.00 24.22 | AAAA |
| ATOM | 2477 | CB | CYS | 311 | 34.297 | 48.097 | 69.343 | 1.00 27.66 1.00 25.37 | AAAA AAAA |
| ATOM | 2478 | SG | CYS | 311 | 34.618 | 49.528 | 68.253 | 1.00 27.22 | AAAA |
| ATOM | 2479 | С | CYS | 311 | 35.224 | | 70.490 | 1.00 22.95 | AAAA |
| ATOM | 2480 | 0 | CYS | 311 | 35.986 | 46.180 | 71.441 | 1.00 25.47 | AAAA |
| ATOM | 2481 | N | GLU | 312 | 34.284 | 45.089 | 70.457 | 1.00 17.03 | AAAA |
| ATOM | 2482 | CA | GLU | 312 | 34.120 | 44.129 | 71.569 | 1.00 22.44 | AAAA |
| ATOM | 2483 | CB | GLU | 312 | 33.011 | 43.110 | 71.280 | 1.00 20.81 | AAAA |
| MOTA MOTA | 2484 2485 | CG CD | GLU | 312 312 | 31.856 32.265 | 43.048 | 72.258 | 1.00 43.65 | AAAA |
| ATOM | 2486 | | GLU | 312 | 33.022 | 42.971 42.059 | 73.717 74.119 | 1.00 29.63 1.00 38.85 | AAAA |
| ATOM | 2487 | | GLU | 312 | 31.804 | 43.844 | 74.473 | 1.00 53.22 | AAAA AAAA |
| ATOM | 2488 | c | GLI | 312 | 35.395 | 43.309 | 71.778 | 1.00 27.47 | AAAA |
| ATOM | 2489 | 0 | GL1. | 312 | 35.899 | 43.178 | 72.895 | 1.00 22.33 | AAAA |
| ATOM | 2490 | N | LEL | 313 | 35.899 | 42.723 | 70.696 | 1.00 23.82 | AAAA |
| MOTA | 2491 | CA | LEU | 313 | 37.101 | 41.889 | 70.771 | 1.00 20.72 | AAAA |
| ATOM | 2492 | CB | LEU | 313 | 37.380 | 41.222 | 69.422 | 1.00 27.82 | AAAA |
| ATOM | 2493 | CG | | 313 | 36.403 | 40.167 | 68.903 | 1.00 33.55 | AAAA |
| ATOM | 2494 | CD1 | LEU | 313 313 | 36.839 | 39.738 | | 1.00 24.03 | AAAA |
| ATOM ATOM | 2495 2496 | CDZ | LEU | 313 | 36.379 38.343 | 38.981 42.670 | 69.846 71.181 | 1.00 28.20 1.00 18.21 | AAAA |
| ATOM | 2497 | ō | LEU | 313 | 39.119 | 42.205 | 72.017 | 1.00 21.48 | AAAA AAAA |
| ATOM | 2498 | N | SER | 314 | 38.492 | 43.848 | 70.580 | 1.00 19.41 | AAAA |
| ATOM | 2499 | CA | SER | 314 | 39.627 | 44.753 | 70.775 | 1.00 28.26 | AAAA |
| ATOM | 2500 | CB | SER | 314 | 39.625 | 45.821 | 69.663 | 1.00 22.55 | AAAA |
| ATOM | 2501 | OG | SER | 314 | 40.732 | 46.696 | 69.759 | 1.00 61.92 | AAAA |
| MOTA | 2502 | С | SER | 314 | 39.619 | 45.429 | 72.144 | 1.00 30.18 | AAAA |
| ATOM | 2503 | 0 | SER | 314 | 40.631 | 45.969 | 72.590 | 1.00 25.04 | AAAA |
| ATOM | 2504 | | GLY | 315 | 38.477 | 45.407 | 72.806 | 1.00 28.04 | AAAA |
| ATOM | 2505 | | GLY | 315 | 38.393 | 46.009 | 74.119 | 1.00 33.84 | AAAA |
| MOTA | 2506 | | GLY | 315 315 | 38.324 | 47.518 | 74.105 | 1.00 36.93 | AAAA |
| ATOM | 2507 | | GLY ARG | 315 316 | 38.811 37.739 | 48.178 | 75.022 | 1.00 37.00 | AAAA |
| ATOM | 2508 | N | TING | 210 | 31.133 | 48.090 | 73.065 | 1.00 31.33 | AAAA . |

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| MOTA | 2509 | CA | ARG | 316 | 37.631 | 49.536 | 73.042 | 1.00 39.10 | AAAA |
|--------------|--------------|-----------|------------|------------|------------------|------------------|------------------|--------------------------|----------------|
| MOTA | 2510 | CB | ARG | 316 | 38.347 | 50.108 | 71.830 | 1.00 45.15 | AAAA |
| MOTA | 2511 | CG | ARG | 316 | 37.722 | 49.834 | 70.501 | 1.00 46.02 | AAAA |
| MOTA | 2512 | CD | ARG | 316 | 38.620 | 50.459 | 69.449 | 1.00 44.83 | AAAA |
| MOTA MOTA | 2513 2514 | NE CZ | ARG ARG | 316 316 | 39.898 40.945 | 49.767 50.219 | 69.357 68.674 | 1.00 37.91 1.00 27.39 | AAAA |
| ATOM | 2515 | CZ | ARG | 316 | 40.854 | 51.371 | 68.034 | 1.00 27.39 | AAAA AAAA |
| ATOM | 2516 | | ARG | 316 | 42.054 | 49.493 | 68.572 | 1.00 34.51 | AAAA |
| ATOM | 2517 | С | ARG | 316 | 36.179 | 49.984 | 73.058 | 1.00 35.43 | AAAA |
| ATOM | 2518 | 0 | ARG | 316 | 35.292 | 49.271 | 72.596 | 1.00 30.71 | AAAA |
| MOTA | 2519 | N | GLU | 317 | 35.931 | 51.162 | 73.612 | 1.00 34.06 | AAAA |
| ATOM | 2520 | CA | GLU | 317 | 34.569 | 51.663 | 73.671 | 1.00 37.96 | AAAA |
| ATOM | 2521 | CB | GLU | 317 | 34.481 | 52.914 | 74.552 | 1.00 43.60 | AAAA |
| ATOM | 2522 | CG | GLU | 317 | 33.961 | 52.630 | 75.960 | 1.00 60.36 | AAAA |
| ATOM ATOM | 2523 2524 | CD | GLU GLU | 317 317 | 34.768 34.375 | 51.575 51.217 | 76.701 77.832 | 1.00 70.70 1.00 76.71 | AAAA AAAA |
| ATOM | 2525 | | GLU | 317 | 35.793 | 51.104 | 76.162 | 1.00 78.36 | AAAA |
| MOTA | 2526 | C | GLU | 317 | 34.068 | 51.958 | 72.280 | 1.00 35.65 | AAAA |
| ATOM | 2527 | O | GLU | 317 | 34.843 | 52.322 | 71.390 | 1.00 32.91 | AAAA |
| ATOM | 2528 | N | VAL | 318 | 32.767 | 51.772 | 72.094 | 1.00 30.52 | AAAA |
| ATOM | 2529 | CA | VAL | 318 | 32.138 | 52.012 | 70.808 | 1.00 37.04 | AAAA |
| ATOM | 2530 | CB | VAL | 318 | 30.877 | 51.138 | 70.638 | 1.00 36.48 | AAAA |
| ATOM | 2531 2532 | | VAL | 318 318 | 30.278 31.222 | 51.366 49.674 | 59.268 70.846 | 1.00 40.43 1.00 33.75 | AAAA AAAA |
| ATOM ATOM | 2532 | C | VAL | 318 | 31.719 | 53.465 | 70.737 | 1.00 28.96 | AAAA |
| ATOM | 2534 | ŏ | VAL | 318 | 30.930 | 53.915 | 71.556 | 1.00 33.56 | AAAA |
| ATOM | 2535 | N | PRO | 319 | 32.258 | 54.229 | 69.773 | 1.00 29.20 | AAAA |
| MOTA | 2536 | CD | PRO | 319 | 33.243 | 53.924 | 68.726 | 1.00 31.62 | AAAA |
| ATOM | 2537 | CA | PRO | 319 | 31.858 | 55.637 | 69.684 | 1.00 28.99 | AAAA |
| ATOM | 2538 | CB | PRO | 319 | 32.709 | 56.154 54.926 | 68.528 | 1.00 32.17 | AAAA |
| ATOM ATOM | 2539 2540 | CG C | PRO PRO | 319 319 | 32.850 30.365 | 55.680 | 67.664 69.377 | 1.00 41.36 1.00 36.95 | AAAA AAAA |
| ATOM | 2541 | Ö | PRO | 319 | 29.847 | 54.795 | 68.695 | 1.00 32.86 | AAAA |
| ATOM | 2542 | N | GLU | 320 | 29.646 | 56.683 | 69.855 | 1.00 34.61 | AAAA |
| MOTA | 2543 | CA | GLU | 320 | 28.230 | 56.657 | 69.544 | 1.00 35.13 | AAAA |
| ATOM | 2544 | CB | GLU | 320 | 27.419 | 57.416 | 70.595 | 1.00 52.97 | AAAA |
| MOTA | 2545 | CG | GLU | 320 | 27.751 | 58.875 | 70.738 | 1.00 56.06 | AAAA |
| ATOM | 2546 2547 | CD OE1 | GLU | 320 320 | 26.822 25.604 | 59.558 59.619 | 71.721 71.444 | 1.00 65.58 1.00 64.27 | AAAA AAAA |
| ATOM ATOM | 2547 | OE2 | GLU GLU | 320 | 27.306 | 60.022 | 72.775 | 1.00 72.99 | AAAA |
| ATOM | 2549 | C | GLU | 320 | 27.943 | 57.192 | 68.153 | 1.00 35.13 | AAAA |
| MOTA | 2550 | 0 | GLU | 320 | 26.916 | 56.879 | 67.565 | 1.00 37.43 | AAAA |
| ATOM | 2551 | N | LYS | 321 | 28.880 | 57.953 | 67.604 | 1.00 28.22 | AAAA |
| MOTA | 2552 | CA | LYS | 321 | 28.700 | 58.555 | 66.289 | 1.00 36.58 | AAAA |
| ATOM | 2553 | CB | LYS | 321 | 28.666 | 60.071 | 66.454 | 1.00 44.87 | AAAA |
| ATOM ATOM | 2554 2555 | CD | LYS | 321 321 | 29.987 30.305 | 60.606 60.020 | 67.023 68.410 | 1.00 55.73 1.00 57.27 | AAA" · AAA: |
| ATOM | 2556 | CE | LYS | 321 | 31.733 | 60.310 | 68.840 | 1.00 54.59 | AAA |
| ATOM | 2557 | NZ | LYS | 321 | 32.024 | 61.774 | 68.848 | 1.00 67.47 | AAAA |
| ATOM | 2558 | С | LYS | 321 | 29.823 | 58.211 | 65.315 | 1.00 34.44 | AAAA |
| ATOM | 2559 | 0 | LYS | 321 | 30.912 | 57.818 | 65.731 | 1.00 33.83 | AAAA |
| MOTA | 2560 | N | LEU | 322 | 29.549 | 58.354 | 64.019 | 1.00 30.21 | AAAA |
| MOTA | 2561 | | LEU | 322 | 30.575 29.966 | 58.135 | 62.998 61.677 | 1.00 29.45 1.00 32.21 | AAAA |
| ATOM | 2562 2563 | CB CG | LEU | 322 322 | 29.240 | 57.677 56.338 | 61.651 | 1.00 32.21 | AAAA AAAA |
| MOTA MOTA | 2564 | CD1 | | 322 | 29.008 | 55.977 | 60.186 | 1.00 38.44 | AAAA |
| ATOM | 2565 | CD2 | | 322 | 30.072 | 55.261 | 62.337 | 1.00 42.11 | AAAA |
| MOTA | 2566 | | LEU | 322 | 31.228 | 59.503 | 62.783 | 1.00 33.28 | AAAA |
| ATOM | 2567 | | LEU | 322 | 30.544 | 60.519 | 62.872 | 1.00 31.45 | AAAA |
| MOTA | 2568 | | ASN | 323 | 32.533 | 59.539 | 62.519 | 1.00 34.38 | AAAA |
| ATOM | 2569 | | ASN | 323 | 33.208 | 60.824 | 62.294 | 1.00 36.53 | AAAA |
| MOTA | 2570 | | ASN | 323 | 34.701 35.484 | 60.737 | 62.600 61.480 | 1.00 42.85 1.00 50.51 | AAAA AAAA |
| ATOM | 2571 2572 | CG OD1 | ASN | 323 323 | 35.404 | 60.081 58.942 | 61.109 | 1.00 50.51 | AAAA |
| ATOM . | 2573 | ND2 | | 323 | 36.455 | 60.807 | 60.928 | 1.00 60.23 | AAAA |
| ATOM | 2574 | | ASN | 323 | 33.027 | 61.171 | 60.822 | 1.00 34.69 | AAAA |

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| ATOM | 2575 | 5 0 | ASN | 323 | 32.42 | 9 60.395 | 60.075 | 1.00 34.06 | AAAA |
|-------|-------|-----|-------|-----|---------|----------|------------------|--------------------------|--------------|
| MOTA | 2576 | 5 N | ASN | 324 | 33.55 | | | | AAAA |
| ATOM | 2577 | | ASN | | 33.38 | | | | AAAA |
| MOTA | 2578 | | | | 33.86 | | | | AAAA |
| ATOM | 2579 | | | | 32.97 | | | | AAAA |
| ATOM | 2580 | | 1 ASN | | 31.76 | | | | AAAA |
| MOTA | 2581 | | 2 ASN | | 33.55 | | | | |
| ATOM | 2582 | | ASN | | 34.04 | | | | AAAA |
| ATOM | 2583 | | ASN | | 33.45 | | | 1.00 24.87 | AAAA |
| ATOM | 2584 | | LYS | | 35.27 | | | 1.00 31.31 | AAAA |
| MOTA | 2585 | | | | - 35.99 | | | | AAAA |
| ATOM | 2586 | | | | 37.35 | | | 1.00 29.55 1.00 37.43 | AAAA |
| ATOM | 2587 | | | | 38.25 | | | 1.00 37.43 | AAAA |
| MOTA | 2588 | | | | 39.684 | | | 1.00 50.89 | AAAA |
| ATOM | 2589 | | | | 40.19 | | | 1.00 54.82 | AAAA |
| ATOM | 2590 | | | | 41.62 | | | | AAAA |
| ATOM | 2591 | | LYS | | 35.16 | | | 1.00 65.70 | AAAA |
| ATOM | 2592 | | LYS | | 35.016 | | | 1.00 27.99 | AAAA |
| ATOM | 2593 | | ALA | | 34.602 | | 58.142 | | AAAA |
| ATOM | 2594 | | ALA | | 33.781 | | | 1.00 26.07 | AAAA |
| ATOM | 2595 | | ALA | | 33.470 | | 58.030 | 1.00 24.38 | AAAA |
| ATOM | 2596 | | ALA | | 32.478 | | 59.428 | 1.00 27.34 | AAAA |
| ATOM | 2597 | o | ALA | 326 | 32.131 | | 57.231 | 1.00 25.78 | AAAA |
| ATOM | 2598 | И | LYS | 327 | 31.749 | | 56.369 | 1.00 27.37 | AAAA |
| ATOM | 2599 | CA | LYS | 327 | 30.502 | | 57.496 | 1.00 27.31 | AAAA |
| ATOM | 2600 | | LYS | 327 | 29.759 | | 56.758 57.313 | 1.00 28.56 | AAAA |
| ATOM | 2601 | CG | LYS | 327 | 29.491 | | 58.812 | 1.00 28.87 | AAAA |
| ATOM | 2602 | CD | LYS | 327 | 28.643 | | 59.255 | 1.00 36.72 | AAAA |
| ATOM | 2603 | CE | LYS | 327 | 28.645 | | 60.769 | 1.00 40.34 1.00 38.91 | AAAA |
| ATOM- | 2604 | NZ | LYS | 327 | 28.163 | | 61.556 | 1.00 38.91 | AAAA |
| ATOM | 2605 | C | LYS | | 30.792 | | 55.269 | 1.00 47.07 | AAAA |
| MOTA | 2606 | ō | LYS | 327 | 30.097 | | 54.393 | 1.00 27.76 | AAAA AAAA |
| ATOM | 2607 | N | GLU | 328 | 31.829 | | 54.972 | 1.00 27.75 | AAAA |
| ATOM | 2608 | CA | GLU | 328 | 32.167 | | 53.581 | 1.00 28.93 | AAAA |
| MOTA | 2609 | CB | GLU | 328 | 33.257 | | 53.515 | 1.00 28.33 | AAAA |
| ATOM | 2610 | CG | GLU | 328 | 32.745 | | 54.067 | 1.00 47.50 | AAAA |
| ATOM | 2611 | CD | GLU | 328 | 33.764 | | 54.032 | 1.00 46.67 | AAAA |
| ATOM | 2612 | OE1 | | 328 | 34.325 | | 52.951 | 1.00 56.88 | AAAA |
| ATOM | 2613 | OE2 | | 328 | 33.984 | | 55.087 | 1.00 42.24 | AAAA |
| ATOM | .2614 | C | GLU | 328 | 32.575 | | 52.871 | 1.00 30.46 | AAAA |
| ATOM | 2615 | 0 | GLU | 328 | 32.226 | | 51.704 | 1.00 26.29 | AAAA |
| ATOM | 2616 | N | LEU | 329 | 33.292 | 58.112 | 53.584 | 1.00 24.93 | AAAA |
| MOTA | 2617 | CA | LEU | 329 | 33.701 | | 53.017 | 1.00 24.80 | AAAA |
| ATOM | 2618 | CB | LEU | 329 | 34.478 | 56.003 | 54.053 | 1.00 25.70 | AAAA |
| ATOM | 2619 | CG | LEU | 329 | 34.730 | 54.522 | 53.703 | 1.00 19.71 | AAAA |
| ATOM | 2620 | CD1 | LEU | 329 | 3.569 | 54.413 | 52.430 | 1.00 25.26 | AAAA |
| MOTA | 2621 | CD2 | LEU | 329 | 55.412 | 53.833 | 54.863 | 1.00 24.73 | AAAA |
| ATOM | 2622 | С | LEU | 329 | 2.443 | 56.059 | 52.603 | 1.00 23.50 | AAAA |
| MOTA | 2623 | 0 | LEU | 329 | 32.310 | 55.650 | 51.453 | 1.00 25.60 | AAAA |
| MOTA | 2624 | N | LEU | 330 | 31.516 | 55.881 | 53.539 | 1.00 23.02 | AAAA |
| ATOM | 2625 | CA | LEU | 330 | 30.289 | 55.145 | 53.242 | 1.00 23.85 | AAAA |
| MOTA | 2626 | CB | LEU | 330 | 29.414 | 55.030 | 54.484 | 1.00 21.74 | AAAA |
| ATOM | 2627 | CG | LEU | 330 | 30.039 | 54.252 | 55.642 | 1.00 25.29 | AAAA |
| ATOM | 2628 | CD1 | LEU | 330 | 28.984 | 54.053 | 56.724 | 1.00 30.58 | . AAAA |
| ATOM | 2629 | CD2 | LEU | 330 | 30.538 | 52.905 | 55.168 | 1.00 22.44 | AAAA |
| ATOM | 2630 | С | LEU | 330 | 29.491 | 55.769 | 52.113 | 1.00 26.94 | AAAA |
| ATOM | 2631 | ö | LEU | 330 | 28.968 | 55.060 | 51.252 | 1.00 26.65 | AAAA |
| ATOM | 2632 | N | LYS | 331 | 29.404 | 57.097 | 52.111 | 1.00 30.82 | AAAA |
| ATOM | 2633 | CA | LYS | 331 | 28.667 | 57.795 | 51.066 | 1.00 29.53 | AAAA |
| ATOM | 2634 | CB | LYS | 331 | 28.537 | 59.292 | 51.407 | 1.00 29.67 | AAAA |
| ATOM | 2635 | CG | LYS | 331 | 27.814 | 59.567 | 52.714 | 1.00 36.06 | AAAA |
| ATOM | 2636 | CD | LYS | 331 | 27.688 | 61.055 | 52.990 | 1.00 42.75 | AAAA |
| ATOM | 2637 | CE | LYS | 331 | 26.828 | 61.737 | 51.939 | 1.00 53.98 | AAAA |
| MOTA | 2638 | NZ | LYS | 331 | 26.634 | 63.185 | 52.234 | 1.00 67.57 | AAAA |
| ATOM | 2639 | c . | LYS | 331 | 29.315 | 57.628 | 49.692 | 1.00 30.07 | AAAA |
| ATOM | 2640 | 0 | LYS | 331 | 28.634 | 57.759 | 48.672 | 1.00 36.20 | AAAA |
| | | | | | | | • | | |

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Figure 16-41

| ATOM | 2641 | N | SER | 332 | 30.608 | 57.305 | 49.657 | 1.00 30.08 | AAAA |
|-------------|------|-----|-------|-------|--------|---------|--------|------------|--------|
| | 2642 | CA | SER | | 31.322 | 57.153 | 48.385 | 1.00 33.35 | |
| ATOM | | | | | | | | | AAAA |
| ATOM | 2643 | CB | SER | | 32.834 | 57.312 | 48.590 | 1.00 40.36 | AAAA |
| ATOM | 2644 | OG | SER | 332 | 33.396 | 56.169 | 49.219 | 1.00 34.04 | AAAA |
| ATOM | 2645 | С | SER | 332 | 31.061 | 55.821 | 47.693 | 1.00 37.72 | AAAA |
| | 2646 | ō | SER | 332 | 31.354 | 55.661 | 46.507 | 1.00 30.78 | |
| ATOM | | | | | | | | 1.00 30.76 | AAAA |
| ATOM | 2647 | N | ILE | 333 | 30.521 | 54.865 | 48.440 | 1.00 30.61 | AAAA |
| MOTA | 2648 | CA | ILE | 333 | 30.219 | 53.547 | 47.899 | 1.00 37.59 | AAAA . |
| MOTA | 2649 | CB | ILE | - 333 | 29.901 | 52.551 | 49.022 | 1.00 33.59 | AAAA |
| - | 2650 | | LILE | 333 | 29.738 | 51.146 | 48.442 | 1.00 37.05 | |
| ATOM | | | | | | | | | AAAA |
| MOTA | 2651 | | . ILE | 333 | 31.015 | 52.564 | 50.065 | 1.00 38.95 | AAAA |
| MOTA | 2652 | CD1 | . ILE | . 333 | 30.706 | 51.727 | 51.282 | 1.00 46.83 | AAAA |
| MOTA | 2653 | С | ILE | 333 | 28.990 | 53.620 | 46.998 | 1.00 43.41 | AAAA |
| ATOM | 2654 | ō | ILE | 333 | 27.889 | 53.876 | 47.479 | 1.00 46.24 | AAAA |
| | | | | | | | | | |
| MOTA | 2655 | N | ASP | 334 | 29.158 | 53.423 | 45.696 | 1.00 47.97 | AAAA |
| ATOM | 2656 | ÇA | ASP | 334 | 27.976 | 53.447 | 44.847 | 1.00 53.47 | - AAAA |
| ATOM | 2657 | CB | ASP | 334 | 28.333 | 53.535 | 43.358 | 1.00 61.52 | AAAA |
| ATOM | 2658 | CG | ASP | 334 | 29.223 | 52.406 | 42.897 | 1.00 64.75 | AAAA |
| | 2659 | | ASP | 334 | 29.379 | 52.248 | 41.666 | 1.00 66.93 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2660 | OD2 | ASP | 334 | 29.779 | 51.691 | 43.758 | 1.00 65.93 | |
| ATOM | 2661 | С | ASP | 334 | 27.248 | 52.144 | 45.161 | 1.00 51.83 | AAAA |
| ATOM | 2662 | 0 | ASP | 334 | 27.626 | 51.067 | 44.699 | 1.00 46.80 | AAAA |
| ATOM | 2663 | N | PHE | 335 | 26.215 | 52.249 | 45.986 | 1.00 54.96 | AAAA |
| | | | | 335 | | • | | | |
| ATOM | 2664 | CA | PHE | | 25.455 | 51.080 | 46.392 | 1.00 50.60 | AAAA |
| ATOM | 2665 | CB | PHE | 335 | 25.413 | 51.003 | 47.920 | 1.00 39.55 | AAAA |
| ATOM | 2666 | CG | PHE | 335 | 24.380 | 50.054 | 48.440 | 1.00 37.98 | AAAA |
| ATOM | 2667 | CD1 | PHE | 335 | 24.389 | 48.715 | 48.054 | 1.00 46.72 | AAAA |
| ATOM | 2668 | | PHE | 335 | 23.362 | 50.506 | 49.262 | 1.00 34.23 | AAAA |
| | | | | | | | 48.478 | | |
| ATOM | 2669 | | PHE | 335 | 23.389 | 47.842 | | 1.00 49.80 | AAAA |
| ATOM | 2670 | CE2 | PHE | 335 | 22.361 | 49.644 | 49.689 | 1.00 48.51 | AAAA |
| ATOM | 2671 | CZ | PHE | 335 | 22.373 | 48.309 | 49.296 | 1.00 40.44 | AAAA |
| ATOM | 2672 | С | PHE | 335 | 24.033 | 51.000 | 45.839 | 1.00 54.52 | AAAA |
| ATOM | 2673 | õ | PHE | 335 | 23.603 | 49.939 | 45.379 | 1.00 59.24 | AAAA |
| | | | | | | | 45.888 | | |
| MOTA | 2674 | N | GLU | 336 | 23.302 | 52.108 | | 1.00 50.94 | AAAA |
| ATOM | 2675 | CA | GLU | 336 | 21.923 | 52.119 | 45.406 | 1.00 57.05 | AAAA |
| ATOM | 2676 | CB | GLU | 336 | 21.853 | 51.751 | 43.924 | 1.00 60.27 | AAAA |
| MOTA | 2677 | CG | GLU | 336 | 20.430 | 51.627 | 43.422 | 1.00 68.55 | AAAA |
| ATOM | 2678 | CD | GLU | 336 | 20.352 | 51.126 | 42.001 | 1.00 80.03 | AAAA |
| | 2679 | | GLU | 336 | 20.860 | 50.013 | 41.735 | 1.00 84.64 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 2680 | | GLU | 336 | 19.777 | 51.841 | 41.153 | 1.00 80.68 | AAAA |
| MOTA | 2681 | С | GLU | 336 | 21.065 | 51.135 | 46.201 | 1.00 55.73 | AAAA |
| MOTA | 2682 | 0 | GLU | 336 | 21.219 | 49.917 | 46.089 | 1.00 51.33 | AAAA |
| ATOM | 2683 | N | GLU | 337 | 20.151 | 51.679 | 46.992 | 1.00 49.54 | AAAA |
| | 2684 | CA | GLU | 337 | 19.267 | 50.880 | 47.821 | 1.00 48.19 | AAAA |
| ATOM | | | | | | | 48.764 | | |
| MOTA | 2685 | CB | GLU | 337 | 18.510 | 51.822 | | 1.00 47.73 | AAAA |
| MOTA | 2686 | CG | GLU | 337 | 18.084 | 51.205 | 50.077 | 1.00 55.69 | AAAA |
| MOTA | 2687 | CD | GLU | . 337 | 19.269 | 50.720 | 50.904 | 1.00 50.17 | AAAA |
| ATOM | 2688 | OE1 | GLU | 337 | 20.111 | 51.548 | 51.345 | 1.00 36.03 | AAAA |
| | 2689 | OE2 | GLU | 337 | 19.358 | 49.494 | 51.105 | 1.00 51.25 | AAAA |
| MOTA | | | | | | | | 1.00 49.13 | |
| ATOM | 2690 | C | GLU | 337 | 18.294 | 50.083 | 46.936 | | AAAA |
| MOTA | 2691 | 0 | GLU | 337 | 17.816 | 50.588 | 45.916 | 1.00 48.61 | AAAA |
| MOTA | 2692 | N | PHE | 338 | 18.015 | 48.837 | 47.313 | 1.00 48.15 | AAAA |
| ATOM | 2693 | CA | PHE | 338 | 17.092 | 48.000 | 46.547 | 1.00 48.12 | AAAA |
| | | | | 338 | 16.870 | 46.658 | 47.249 | 1.00.54.54 | AAAA |
| MOTA | 2694 | CB | PHE | | | | | | |
| ATOM | 2695 | CG | PHE | 338 | 15.883 | 45.777 | 46.548 | 1.00 57.22 | AAAA |
| ATOM: | 2696 | CD1 | PHE | 338 | 16.115 | 45.366 | 45.243 | 1.00 60.01 | AAAA |
| ATOM | 2697 | | PHE | 338 | 14.699 | 45.398 | 47.171 | 1.00 55.04 | AAAA |
| | 2698 | CE1 | | 338 | 15.185 | 44.597 | 44.566 | 1.00 60.84 | AAAA |
| ATOM | | | | 338 | 13.758 | | 46.497 | 1.00 59.41 | AAAA |
| MOTA | 2699 | CE2 | | | | 44.624 | | | |
| MOTA | 2700 | CZ | PHE | 338 | 14.002 | 44.224 | 45.189 | 1.00 57.18 | AAAA |
| ATOM | 2701 | С | PHE | 338 | 15.755 | 48.714 | 46.380 | 1.00 45.46 | AAAA |
| ATOM | 2702 | o | PHE | 338 | 15.274 | 48.900 | 45.263 | 1.00 51.11 | AAAA |
| | 2703 | N | ASP | 339 | 15.154 | 49.098 | 47.501 | 1.00 40.38 | AAAA |
| ATOM | | | | 339 | 13.890 | | 47.488 | 1.00 49.97 | AAAA |
| ATOM · | 2704 | CA | ASP | | | 49.820. | | | |
| MOTA | 2705 | CB | ASP | 339 | 13.270 | 49.821 | 48.886 | 1.00 53.23 | AAAA |
| ATOM | 2706 | CG | ASP | 339 | 12.000 | 50.659 | 48.968 | 1.00 57.40 | AAAA |

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Figure 16-42

| | • | | | | | | | | |
|--------------|--------------|----------|--------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 2707 | | 1 ASP | | 12.039 | | 48.616 | 1.00 53.79 | AAAA |
| ATOM | 2708 | | 2 ASP | | 10.963 | 50.118 | | 1.00 51.15 | AAAA |
| MOTA | 2709 | С | ASP | | 14.215 | 51.248 | | 1.00 55.06 | AAAA |
| MOTA | 2710 | 0 | ASP | | 14.994 | 51.922 | 47.748 | 1.00 56.47 | AAAA |
| MOTA | 2711 | N | ASP | | 13.623 | 51.708 | 45.978 | 1.00 58.46 | AAAA |
| ATOM | 2712 | CA | | | 13.874 | 53.059 | 45.484 | 1.00 67.72 | AAAA |
| MOTA | 2713 | CB | ASP | | 12.683 | 53.559 | 44.664 | 1.00 71.52 | AAAA |
| MOTA | 2714 | CG | ASP | | 12.611 | 52.913 | 43.295 | 1.00 79.72 | AAAA |
| ATOM | 2715 | | 1 ASP | | 12.528 | 51.667 | 43.224 | 1.00 86.74 | AAAA |
| MOTA | 2716 | | 2 ASP | | 12.640 | 53.655 | 42.288 | 1.00 83.40 | AAAA |
| MOTA | 2717 | C | ASP | | 14.209 | 54.072 | 46.572 | 1.00 69.65 | AAAA |
| MOTA | 2718 | 0 | ASP | | 15.204 | 54.794 | 46.463 | 1.00 70.13 | AAAA |
| ATOM | 2719 | N | GLU | | 13.392 | 54.130 | 47.620 | 1.00 67.11 | AAAA |
| MOTA | 2720 | CA | GLU | | 13.668 | 55.077 | 48.689 | 1.00 67.87 | AAAA |
| ATOM | 2721 | CB | GLU | | 13.195 13.502 | 56.478 | 48.278 | 1.00 74.87 | AAAA |
| MOTA | 2722 2723 | CG | GLU | | | 57.576 | 49.298 | 1.00 82.72 | AAAA |
| MOTA | 2724 | CD | GLU 1 GLU | | 13.162 11.988 | 58.974 | 48.790 | 1.00 90.80 | AAAA |
| MOTA MOTA | 2725 | | 2 GLU | | 14.072 | 59.215 59.835 | 48.431 48.752 | 1.00 90.38 | AAAA |
| MOTA | 2726 | C | GLU | 341 | 13.101 | 54.719 | 50.058 | 1.00 93.36 | AAAA |
| ATOM | 2727 | ō | GLU | 341 | 11.929 | 54.955 | 50.347 | 1.00 60.22 1.00 58.81 | AAAA |
| ATOM | 2728 | N | VAL | 342 | 13.956 | 54.144 | 50.897 | 1.00 57.28 | AAAA |
| ATOM | 2729 | CA | VAL | 342 | 13.594 | 53.781 | 52.262 | 1.00 52.09 | AAAA AAAA |
| ATOM | 2730 | CB | VAL | 342 | 14.195 | 52.419 | 52.669 | 1.00 53.17 | AAAA |
| MOTA | 2731 | | VAL | 342 | 13.730 | 52.042 | 54.070 | 1.00 46.16 | AAAA |
| ATOM | 2732 | | VAL | 342 | 13.815 | 51.356 | 51.663 | 1.00 59.09 | AAAA |
| ATOM | 2733 | C | VAL | 342 | 14.263 | 54.843 | 53.124 | 1.00 53.31 | AAAA |
| ATOM | 2734 | 0 | VAL | 342 | 13.763 | 55.230 | 54.185 | 1.00 57.79 | AAAA |
| ATOM | 2735 | N | ASP | 343 | 15.398 | 55.306 | 52.610 | 1.00 46.24 | AAAA |
| ATOM | 2736 | CA | ASP | 343 | 16.268 | 56.289 | 53.243 | 1.00 42.60 | AAAA |
| ATOM | 2737 | CB | ASP | 343 | 15.521 | 57.510 | 53.781 | 1.00 43.88 | AAAA |
| ATOM | 2738 | CG | ASP | 343 | 16.480 | 58.581 | 54.290 | 1.00 46.82 | AAAA |
| MOTA | 2739 | | ASP | 343 | 16.028 | 59.581 | 54.887 | 1.00 46.16 | AAAA |
| MOTA | 2740 | | ASP | 343 | 17.700 | 58.414 | 54.075 | 1.00 33.01 | AAAA |
| MOTA | . 2741 | С | ASP | 343 | 17.012 | 55.636 | 54.395 | 1.00 35.45 | AAAA |
| ATOM | 2742 | 0 | ASP | 343 | 16.487 | 55.480 | 55.502 | 1.00 29.39 | AAAA |
| ATOM | 2743 | N | ARG | 344 | 18.247 | 55.249 | 54.124 | 1.00 30.51 | AAAA |
| ATOM | 2744 2745 | CA CB | ARG | 344 | 19.059 | 54.613 | 55.140 | 1.00 29.43 | AAAA |
| ATOM ATOM | 2745 | CG | ARG | 344 344 | 19.736 18.803 | 53.377 52.258 | 54.561 54.180 | 1.00 30.10 1.00 33.95 | AAAA |
| ATOM | 2747 | CD | ARG | 344 | 17.981 | 51.770 | 55.365 | 1.00 33.93 | AAAA AAAA |
| ATOM | 2748 | NE | ARG | 344 | 17.120 | 50.673 | 54.936 | 1.00 20.32 | AAAA |
| ATOM | 2749 | cz | ARG | 344 | 16.110 | 50.176 | 55.639 | 1.00 29.13 | AAAA |
| ATOM | 2750 | | ARG | 344 | 15.805 | 50.668 | 56.835 | 1.00 29.63 | AAAA |
| MOTA | 2751 | | ARG | 344 | 15.379 | 49.198 | 55.120 | 1.00 27.19 | AAAA |
| ATOM | 2752 | С | ARG | 344 | 20.116 | 55.769 | 55.660 | 1.00 34.31 | AAAA |
| ATOM | 2753 | 0 | ARG | 344 | 21.005 | 5557 | 56.391 | 1.00 29.09 | AAAA |
| ATOM | 2754 | N | SER | 345 | 20.011 | 56. 45 | 55.294 | 1.00 28.34 | AAAA |
| MOTA | 2755 | CA | SER | 345 | 20.999 | 57.839 | 55.715 | 1.00 30.95 | AAAA |
| ATOM | 2756 | CB | SER | 345 | 20.669 | 59.199 | 55.109 | 1.00 29.56 | AAAA |
| MOTA | 2757 | OG | SER | 345 | 19.429 | 59.648 | 55.610 | 1.00 29.38 | AAAA |
| MOTA | 2758 | C | SER | 345 | 21.137 | 57.988 | 57.230 | 1.00 30.92 | AAAA |
| MOTA | 2759 | 0 | SER | 345 | 22.155 | 58.488 | 57.718 | 1.00 31.15 | AAAA |
| MOTA | 2760 | N | TYR | 346 | 20.116 | 57.576 | 57.975 | 1.00 25.64 | AAAA |
| ATOM | 2761 | CA | TYR | 346 | 20.158 | 57.659 | 59.433 | 1.00 26.81 | AAAA |
| MOTA | 2762 | CB | TYR | 346 | 18.823 | 57.189 | 60.006 | 1.00 34.41 | AAAA |
| MOTA | 2763 | CG | TYR | 346 | 18.529 | 55.723 | 59.716 | 1.00 27.35 | AAAA |
| ATOM | 2764 2765 | | TYR | 346 | 19.003 18.744 | 54.708 | 60.556 | 1.00 24.87 | AAAA |
| ATOM | | | TYR | 346 | 18.744 | 53.352 | 60.278 | 1.00 28.05 | AAAA |
| ATOM | 2766 2767 | | TYR | 346 346 | 17.795 | 55.358 | 58.588 | 1.00 27.70 1.00 26.59 | AAAA |
| ATOM | 2768 | | TYR | 346 346 | 18.008 | 54.008 53.015 | 58.297 59.145 | 1.00 26.39 | AAAA AAAA |
| atom atom | 2768 2769 | CZ OH | TYR TYR | 346 | 17.737 | 51.691 | 58.855 | 1.00 33.75 | AAAA |
| ATOM . | 2770 | C | TYR | 346 | 21.277 | 56.766 | 59.977 | 1.00 25.57 | AAAA |
| ATOM | 2771 | 0 | TYR | 346 | 21.769 | 56.970 | 61.085 | 1.00 28.07 | AAAA |
| ATOM | 2772 | N . | MET | 347 | 21.666 | 55.761 | 59.198 | 1.00 29.08 | AAAA |
| | | | | | | J , U L | | | |

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| MOTA | 2773 | CA | MET | 347 | 22. | 720 | 54.837 | 59.622 | 1.00 | 24.19 | AAAA |
|-------------------|-------------------|-----|-----|------|-----|-----|--------|--------|--------|-------|------|
| | | CB | MET | 347 | 22. | | 53.678 | 58.628 | 1.00 | 24.87 | AAAA |
| ATOM | 2774 | | | | | | | 58.543 | | 23.66 | AAAA |
| ATOM | 2775 | CG | MET | 347 | 21. | | 52.806 | | | | |
| ATOM | 2776 | SD | MET | 347 | 21. | 780 | 51.503 | 57.267 | 1.00 | 27.02 | AAAA |
| | 2777 | CE | MET | 347 | 22. | 115 | 52.375 | 55.896 | 1.00 | 37.69 | AAAA |
| ATOM | | | | | | | | | | 29.45 | AAAA |
| ATOM | 2778 | С | MET | 347 | 24. | 054 | 55.540 | 59.737 | | | |
| ATOM | 2779 | 0 | MET | 347 | 24. | 937 | 55.092 | 60.479 | 1.00 | 28.08 | AAAA |
| | | | | | 24. | | 56.650 | 59.007 | 1 00 | 23.71 | AAAA |
| ATOM | 2780 | N | LEU | 348 | | | | | | | |
| MOTA | 2781 | CA | LEU | 348 | 25. | 418 | 57.446 | 58.998 | 1.00 | 34.11 | AAAA |
| ATOM | 2782 | CB | LEU | 348 | 25. | 463 | 58.351 | 57.757 | 1.00 | 25.37 | AAAA |
| | | | | | 25. | | 57.785 | 56.344 | 1 00 | 30.38 | AAAA |
| ATOM | 2783 | CG | LEU | 348 | | | | | | | |
| ATOM | 2784 | CD1 | LEU | 348 | 25. | 307 | 58.944 | 55.340 | 1.00 | 27.44 | AAAA |
| ATOM | 2785 | CD2 | LEU | 348 | 26. | 459 | 56.814 | 56.041 | 1.00 | 36.44 | AAAA |
| | | | | | 25. | | 58.332 | 60.237 | 1 00 | 36.09 | AAAA |
| MOTA | 2786 | С | LEU | 348 | | | | | | | |
| ATOM | 2787 | 0 | LEU | 348 | 26. | 561 | 58.894 | 60.539 | | 33.30 | AAAA |
| ATOM | 2788 | N | GLU | 349 | 24. | 394 | 58.445 | 60.953 | 1.00 | 30.51 | AAAA |
| | | | | | 24. | | 59.292 | 62.136 | 1 00 | 35.53 | AAAA |
| MOTA | 2789 | CA | GLU | 349 | _ | | | | | | |
| ATOM | 2790 | CB | GLU | 349 | 22. | 908 | 59.896 | 62.217 | | 31.35 | AAAA |
| ATOM | 2791 | CG | GLU | 349 | 22. | 518 | 60.717 | 61.006 | 1.00 | 29.09 | AAAA |
| | | | | | 23. | | 61.859 | 60.746 | 1 00 | 31.78 | AAAA |
| ATOM | 2792 | CD | GLU | 349 | | | | | | | |
| ATOM | 27 9 3 | OE1 | GLU | 349 | 23. | 937 | 62.476 | 61.730 | | 30.98 | AAAA |
| MOTA | 2794 | OE2 | GLU | 349 | 23. | 766 | 62.155 | 59.569 | 1.00 | 30.67 | AAAA |
| | | | | 349 | 24. | | 58,633 | 63.471 | 1.00 | 38.48 | AAAA |
| MOTA | 2795 | C | GLU | | | | | | | 40.12 | AAAA |
| MOTA | 2796 | 0 | GLU | 349 | 24. | | 59.303 | 64.502 | | | |
| MOTA | 2797 | N | THR | 350 | 24. | 878 | 57.326 | 63.461 | 1.00 | 33.58 | AAAA |
| | 2798 | CA | THR | 350 | 25. | | 56.612 | 64.681 | 1.00 | 29.74 | AAAA |
| MOTA | | | | | | | | 65.559 | | 35.91 | AAAA |
| MOTA | 2799 | CB | THR | 350 | 23. | | 56.363 | | | | |
| ATOM | 2800 | OG1 | THR | 350 | 23. | 421 | 57.615 | 65.952 | 1.00 | 45.03 | AAAA |
| - | 2801 | CG2 | THR | 350 | 24. | 382 | 55.586 | 66.806 | 1.00 | 49.48 | AAAA |
| ATOM | | | | | 25. | | 55.267 | 64.330 | | 30.63 | AAAA |
| ATOM | 2802 | С | THR | 350 | | | | | | | |
| ATOM | 2803 | 0 | THR | 350 | 25. | 535 | 54.709 | 63.274 | | 26.62 | AAAA |
| ATOM | 2804 | N | LEU | 351 | 26. | 644 | 54.740 | 65.225 | 1.00 | 29.07 | AAAA |
| | | | | 351 | 27. | | 53.461 | 64.972 | 1.00 | 24.59 | AAAA |
| MOTA | 2805 | CA | LEU | | | | - | 65.757 | | 29.91 | AAAA |
| ATOM | 2806 | CB | LEU | 351 | 28. | | 53.367 | | | | |
| ATOM | 2807 | CG | LEU | 351 | 29. | 591 | 52.327 | 65.267 | | 39.62 | AAAA |
| | 2808 | | LEU | 351 | 30. | 887 | 52.467 | 66.039 | 1.00 | 37.09 | AAAA |
| MOTA | | | | | 29. | | 50.935 | 65.415 | 1 00 | 54.03 | AAAA |
| ATOM | 2809 | | LEU | 351 | | | | | | | AAAA |
| MOTA | 2810 | C | LEU | 351 | 26. | 314 | 52.336 | 65.377 | | 29.71 | |
| ATOM | 2811 | 0 | LEU | 351 | 26. | 130 | 51.364 | 64.641 | 1.00 | 30.53 | AAAA |
| | | | | 352 | 25. | 697 | 52.481 | 66.543 | 1.00 | 28.64 | AAAA |
| MOTA | 2812 | N | LYS | | | | | 67.061 | | 32.72 | AAAA |
| ATOM | 2813 | CA | LYS | 352 | 24. | | 51.479 | | | | |
| ATOM | 2814 | CB | LYS | 352 | 24. | 913 | 51.381 | 68.581 | 1.00 | 27.37 | AAAA |
| | 2815 | CG | LYS | 352 | 26. | 230 | 50.787 | 69.034 | 1.00 | 43.48 | AAAA |
| ATOM | | | | | 26. | | 51.068 | 70.504 | 1 00 | 46.77 | AAAA |
| MOTA | 2816 | CD | LYS | 352 | | | | | | | AAAA |
| MOTA | 2817 | CE | LYS | 352 | 25. | 484 | 50.538 | 71.451 | | 51.52 | |
| A OM | 2818 | NZ | LYS | 352 | 25. | 850 | 50.859 | 72.866 | 1.00 | 62.08 | AAAA |
| | | C | LYS | 352 | 23. | 330 | 51.856 | 66.731 | 1.00 | 32.49 | AAAA |
| A 1'OM | 2819 | | | | | | | | | 31.90 | AAAA |
| A ₁ OM | 2820 | 0 | LYS | 352 | 22. | | 53.010 | 66.882 | | | |
| ATOM | 2821 | N | ASP | 353 | 22. | 525 | 50.916 | 66.244 | | 31.44 | AAAA |
| ATOM | 2822 | CA | ASP | 353 | 21. | 136 | 51.286 | 66.012 | | 26.50 | AAAA |
| | | | | 353 | 20. | | 50.635 | 64.746 | 1 00 | 50.09 | AAAA |
| MOTA | 2823 | CB | ASP | | | | | | | | AAAA |
| MOTA | 2824 | CG | ASP | 353 | 20. | 880 | 49.176 | 64.604 | . 1.00 | | |
| ATOM | 2825 | 001 | ASP | 353 | 21. | 980 | 48.861 | 64.109 | 1.00 | 58.55 | AAAA |
| | | | | 353 | 20. | | 48.339 | 64.984 | 1.00 | 73.19 | AAAA |
| ATOM | 2826 | | ASP | | | | | | | 26.41 | AAAA |
| MOTA | 2827 | С | ASP | 353 | 20. | | 50.930 | 67.257 | | | |
| ATOM | 2828 | 0 | ASP | 353 | 20. | 806 | 50.214 | 68.136 | | 25.73 | AAAA |
| | | | | 354 | 19. | | 51.481 | 67.385 | 1.00 | 30.12 | AAAA |
| MOTA | 2829 | N | PRO | | | | | 66.495 | | 35.38 | AAAA |
| ATOM | 2830 | CD | PRO | 354 | 18. | | 52.429 | | | | |
| ATOM | 2831 | CA | PRO | 354 | 18. | 276 | 51.190 | 68.547 | | 34.02 | AAAA |
| | | | PRO | 354 | 17. | | 52.129 | 68.340 | 1.00 | 32.25 | AAAA |
| MOTA | 2832 | CB | | | | | | 66.833 | | 44.48 | AAAA |
| ATCM | 2833 | CG | PRO | 354 | 16. | | 52.139 | | | | |
| ATOM | 2834 | C | PRO | 354 | 17. | 838 | 49.736 | 68.512 | | 34.00 | AAAA |
| | | ō | PRO | 354 | 17. | 829 | 49.111 | 67.452 | | 28.28 | AAAA |
| ATOM | 2835 | | | | 17. | | | 69.664 | | 23.89 | AAAA |
| ATOM | 2836 | Ŋ | TRP | 355 | | | 49.190 | | | | AAAA |
| ATOM | 2837 | CA | TRP | 355. | 17. | 010 | 47.818 | 69.669 | | 33.84 | |
| | 2838 | CB | TRP | 355 | 16. | 653 | 47.363 | 71.076 | 1.00 | 33.84 | AAAA |
| ATOM | 2030 | ٠. | | · | | | | - | | | • |
| | | • | | | | | | | | | |

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Figure 16-44

| MOTA | 283 <i>9</i> | CG | TRP | 355 | 17.844 | 46.946 | | 1.00 49.97 | AAAA |
|--------------|--------------|------------------|-------|------|----------|--------|---------|------------|--------------|
| ATOM | 2840 | CD2 | TRP | 355 | 18.364 | 45.622 | 71.905 | 1.00 46.60 | AAAA |
| | | | | | | | | | |
| ATOM | 2841 | CEZ | | | 19.567 | | 72.639 | 1.00 54.73 | AAAA |
| ATOM | 2842 | CE3 | TRP | 355 | 17.931 | 44.386 | 71.419 | 1.00 46.90 | AAAA |
| ATOM | 2843 | CD1 | TRP | 355 | 18.723 | 47.746 | | 1.00 56.10 | AAAA |
| | | | | | | | | | |
| ATOM | 2844 | | . TRP | | 19.765 | | | 1.00 56.07 | AAAA |
| ATOM | 2845 | CZ2 | TRP | 355 | 20.340 | 44.552 | 72.897 | 1.00 55.25 | AAAA |
| ATOM | 2846 | C2.3 | TRP | 355 | 18.696 | 43.267 | 71.674 | 1.00 50.74 | AAAA |
| | | | | | | | | | |
| MOTA | 2847 | CH2 | | | 19.887 | | 72.405 | 1.00 50.68 | AAAA |
| ATOM | 2848 | C | TRP | 355 | 15.789 | 47.712 | 68.776 | 1.00 33.12 | AAAA |
| MOTA | 2849 | 0 | TRP | 355 | . 15.096 | 48.705 | 68.550 | 1.00 29.41 | AAAA |
| | | | | | | | | | |
| ATOM | 2850 | N | ARG | | 15.547 | 46.508 | 68.263 | 1.00 23.90 | AAAA. |
| ATOM | 2851 | CA | ARG | 356 | 14,413 | 46.237 | 67.387 | 1.00 23.96 | AAAA |
| MOTA | 2852 | CB | ARG | 356 | 14.892 | 46.096 | 65 935 | 1.00 22.66 | |
| | | | | | 15.505 | 47.385 | 65.393 | | |
| MOTA | 2853 | CG | ARG | | | | 05.393 | 1.00 29.06 | AAAA |
| MOTA | 2854 | CD | ARG | 356 | 16.291 | 47.212 | 64.108 | 1.00 28.92 | AAAA |
| ATOM | 2855 | NE | ARG | 356 | 16.833 | 48.503 | 63.686 | 1.00 24.73 | AAAA |
| ATOM | 2856 | CZ | ARG | 356 | 17.733 | 48.668 | 62.724 | 1.00 23.57 | |
| | | | | | | | | | AAAA |
| ATOM | 2857 | NHI | ARG | 356 | 18.209 | 47.616 | 62.066 | 1.00 22.15 | AAAA |
| ATOM | 2858 | NH2 | ARG | 356 | 18.153 | 49.891 | 62.418 | 1.00 22.69 | AAAA |
| ATOM | 2859 | С | ARG | 356 | 13.781 | 44.944 | 67.878 | 1.00 24.89 | AAAA |
| | | | | | | | | | |
| ATOM | 2860 | 0 | ARG | 356 | 13.785 | 43.925 | 67.189 | 1.00 22.25 | AAAA |
| ATOM | 2861 | N | GLY | 357 | 13.231 | 44.993 | 69.085 | 1.00 23.91 | AAA:A |
| ATOM | 2862 | CA | GLY | 357 | 12.631 | 43.805 | 69.657 | 1.00 26.72 | AAAA |
| | | | | | | | | | |
| ATOM | 2863 | С | GLY | 357 | 11.138 | 43.671 | 69.465 | 1.00 26.90 | AAAA |
| ATOM | 2864 | 0 | GLY | 357 | 10.536 | 44.330 | 68.619 | 1.00 29.87 | AAAA |
| MOTA | 2865 | N | GLY | 358 | 10.544 | 42.797 | 70.265 | 1.00 28.22 | AAAA |
| ATOM | 2866 | CA | GLY | 358 | 9.118 | 42.561 | 70.188 | | |
| | | | | | | | | 1.00 30.96 | AAAA |
| ATOM | 2867 | С | GLY | 358 | 8.800 | 41.274 | 70.920 | 1.00 30.03 | KAA A |
| ATOM | 2868 | 0 | GLY | 358 | 9.626 | 40.757 | 71.663 | 1.00 24.03 | AAAA |
| MOTA | 2869 | N | GLU | 359 | 7.601 | 40.747 | 70.715 | 1.00 28.34 | AAAA |
| | | | | | | | | | |
| ATOM | 2870 | CA | GLU | 359 | 7.218 | 39.509 | 71.366 | 1.00 24.37 | AAAA |
| ATOM | 2871 | $^{\mathtt{CB}}$ | GLU | 359 | 5.699 | 39.372 | 71.375 | 1.00 32.52 | AAAA |
| ATOM | 2872 | CG | GLU | 359 | 4.981 | 40:327 | 72.299 | 1.00 45.44 | AAAA |
| ATOM | 2873 | CD | GLU | 359 | 3.472 | 40.250 | 72.132 | 1.00 50.43 | AAAA |
| | | | | | | | | | |
| MOTA | 2874 | | GLU | 359 | 2.924 | 39.125 | 72.151 | 1.00 42.92 | AAAA |
| ATOM | 2875 | OE2 | GLU | 359 | 2.839 | 41.316 | 71.987 | 1.00 40.72 | AAAA |
| ATOM | 2876 | C | GLU | 359 | 7.804 | 38.323 | 70.628 | 1.00 27.35 | AAAA |
| ATOM | 2877 | ō | | 359 | 8.138 | 38.415 | 69.449 | | AAAA |
| | | | GLU | | | | | 1.00 22.94 | |
| A TOM | 2878 | N | VAL | 360 | 7.944 | 37.208 | 71.325 | 1.00 19.68 | AAAA |
| ATOM | 2879 | CA | VAL | 360 | 8.441 | 36.017 | 70.672 | 1.00 21.28 | AAAA |
| ATOM | 2880 | CB | VAL | 360 | 9.300 | 35.188 | 71.621 | 1.00 26.71 | AAAA |
| ATOM | 2881 | | VAL | 360 | 9.783 | 33.917 | 70.912 | | AAAA |
| | | | | | | | 70.312 | 1.00 20.64 | |
| MOTA | 2882 | CG2 | VAL | 360 | 10.486 | 36.038 | 72.113 | 1.00 25.79 | AAAA |
| MOTA | 2883 | С | VAL | 360 | 7.228 | 35.202 | 70.197 | 1.00 25.51 | AAAA |
| MOTA | 2884 | 0 | VAL | 360 | 6.442 | 34.700 | 71.011 | 1.00 19.75 | AAAA |
| | | | | | 7.065 | 35.094 | 68.87.3 | | AAAA |
| MOTA | 2885 | N | ARG | 361 | | | | 1.00 18.48 | |
| ATOM | 2886 | CA | ARG | 361 | 5.947 | 34.337 | 68.3¢` | 1.00 22.01 | AAAA |
| ATOM | 2887 | CB | ARG | 361 | 5.988 | 34.389 | 66.772 | 1.00 19.31 | AAAA |
| ATOM | 2888 | CG | ARG | 361 | 5446 | 35.671 | 66.204 | 1.00 30.86 | AAAA |
| | | | | | | | | | |
| ATOM | 2889 | CD | ARG | 361 | 5.735 | 35.730 | 64.723 | 1.00 37.95 | AAAA |
| MOTA | 2890 | NE | ARG | 361 | 7.111 | 36.148 | 64.460 | 1.00 30.73 | AAAA. |
| MOTA | 2891 | CZ | ARG | 361 | 7.616 | 36.275 | 63.242 | 1.00 22.89 | AAAA |
| | | | | | | | | | |
| MOTA | 2892 | NHl | | 361 | 6.851 | 36.006 | 62.186 | 1.00 19.02 | AAAA |
| ATOM | 2893 | NH2 | ARG | 361 | 8.861 | 36.704 | 63.081 | 1.00 23.47 | AAAA |
| MOTA | 2894 | C | ARG | 361 | 5.897 | 32.879 | 68.714 | 1.00 26.11 | AAAA |
| | | | | | 6.926 | 32.255 | 68.968 | 1.00 21.79 | AAAA |
| ATOM | 2895 | | ARG | 361 | | | | | |
| ATOM | 2896 | N | LYS | 362 | 4.681 | 32.338 | 68.763 | 1.00 24.89 | AAAA |
| MOTA | 2897 | | LYS | 362 | 4.479 | 30.938 | 69.125 | 1.00 28.63 | AAAA |
| ATOM | 2898 | | LYS | 362 | 2.981 | 30.570 | 69.070 | 1.00 22.91 | AAAA |
| | | | | | | | | | |
| ATOM | 2899 | | LYS | 362 | 2.145 | 31.200 | 70.168 | 1.00 50.86 | AAAA |
| MOTA | 2900 | CD | LYS | 362 | 2.290 | 32.715 | 70.157 | 1.00 57.51 | AAAA |
| ATOM | 2901 | | LYS | 362 | 1.923 | 33.278 | 68.799 | 1.00 50.87 | AAAA |
| | | | | | 2.307 | 34.683 | 68.711 | 1.00 22.99 | AAAA |
| ATOM | 2902 | | LYS | 362 | | | | | |
| ATOM | 2903 | С | LYS | 362 | 5.269 | 30.014 | 68.202 | 1.00 16.77 | AAAA |
| ATOM | 2904 | 0 | LYS | 3.62 | 5.808 | 29.007 | 68.647 | 1.00 22.90 | AAAA |
| | | - | - | | | | - | | |

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Figure 16-45

| ATOM | 2905 | N | GLU | 363 | 5.311 | 30.355 | 66.913 | 1.00 25.24 | AAAA |
|--------|--------|------|-----|------|--------|--------|---------|------------|-------------|
| ATOM | 2906 | CA | GLU | 363 | 6.055 | 29.577 | 65.910 | 1.00 26.29 | AAAA |
| | 2907 | СВ | GLU | | 6.207 | 30.342 | 64.608 | 1.00 33.50 | |
| ATOM | | | | | | | | | AAAA |
| MOTA | 2908 | CG | GLU | 363 | 4.999 | 30.639 | 63.824 | 1.00 48.73 | AAAA |
| ATOM | 2909 | CD | GLU | 363 | 5.368 | 31.494 | 62.638 | 1.00 42.01 | Aaaa |
| ATOM - | 2910 | OE | GLU | 363 | 6.299 | 31.087 | 61.895 | 1.00 28.50 | AAAA |
| | | | | | | | | | |
| MOTA | · 2911 | OE2 | | | 4.738 | 32.558 | 62.461 | 1.00 44.91 | AAAA |
| ATOM | 2912 | С | GLU | 363 | 7.481 | 29.326 | 66.349 | 1.00 19.00 | Aaaa |
| MOTA | 2913 | 0 | GLU | 363 | 8.011 | 28.218 | 66.226 | 1.00 18.66 | AAAA |
| | | | | 364 | 8.121 | 30.399 | 66.790 | 1.00 20.69 | |
| MOTA | 2914 | 17 | VAL | | | | | | AAAA |
| MOTA | 2915 | CA | VAL | 364 | 9.501 | 30.303 | 67.219 | 1.00 23.13 | AAAA |
| MOTA | 2916 | CB | VAL | .364 | 10.096 | 31.681 | 67.510 | 1.00 16.98 | AAAA |
| MÓTA | 2917 | | VAL | 364 | 11.515 | 31.513 | 68.010- | | AAAA |
| | | | | | 10.082 | 32.548 | 66.242 | 1.00 23.99 | |
| MOTA | 2918 | | VAL | 364 | | | | | AAAA |
| MOTA | 2919 | C, | VAL | 364 | 9.625 | 29.415 | 68.448 | 1.00 19.28 | AAAA |
| ATOM | 2920 | 0 | VAL | 364 | 10.507 | 28.548 | 68.510 | 1.00 20.17 | - Aaaa |
| ATOM | 2921 | | LYS | 365 | 8.735 | 29.600 | 69.417 | 1.00 21.11 | AAAA |
| | | | | | | | | | |
| MOTA | 2922 | CA | LYS | 365 | 8.780 | 28.768 | 70.612 | 1.00 18.15 | AAAA |
| ATOM | 2923 | CB | LYS | 365 | 7.711 | 29.210 | 71.626 | 1.00 25.22 | AAAA |
| MOTA | 2924 | CG | LYS | 365 | 7.921 | 30.611 | 72.167 | 1.00 32.99 | SAAA |
| | 2925 | CD | LYS | 365 | 6.901 | 30.949 | 73.253 | 1.00 36.09 | AAAA |
| MOTA | | | | | | | | | |
| MOTA | 2926 | CE | LYS | 365 | 7.121 | 32.357 | 73.790 | 1.00 28.99 | AAAA |
| ATOM | 2927 | NZ | LYS | 365 | 6.178 | 32.736 | 74.882 | 1.00 38.98 | AAAA |
| ATOM | 2928 | С | LYS | 365 | 8.574 | 27.305 | 70.236 | 1.00 19.49 | AAAA |
| | 2929 | ō | LYS | 365 | 9.255 | 26.417 | 70.758 | 1.00 22.04 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 2930 | N | ASP | 366 | 7.635 | 27.048 | 69.327 | 1.00 22.45 | AAAA |
| ATOM | 2931 | CÀ | asp | 366 | 7.386 | 25.669 | 68.915 | 1.00 22.62 | AAAA |
| MOTA | 2932 | CB | ASP | 366 | 6.173 | 25.574 | 67.967 | 1.00 21.69 | AAAA |
| ATOM | 2933 | CG | ASP | 366 | 4.870 | 25.987 | 68.634 | 1.00 27.75 | AAAA |
| | | | | | | | | | |
| MOTA | 2934 | | ASP | 366 | 4.763 | 25.890 | 69.881 | 1.00 31.01 | AAAA |
| ATOM | 2935 | CD2 | ASP | 366 | 3.938 | 26.382 | 67.907 | 1.00 33.20 | AAAA |
| ATOM | 2936 | С | ASP | 366 | 8.606 | 25.034 | 68.237 | 1.00 24.53 | AAAA |
| ATOM | 2937 | ō | ASP | 366 | 8.924 | 23.871 | 68.480 | 1.00 21.13 | AAAA |
| | | | | | | | 67.380 | | |
| ATOM | 2938 | Ŋ | THR | 367 | 9.281 | 25.787 | | 1.00 26.19 | AAAA |
| ATOM | 2939 | CA | THR | 367 | 10.462 | 25.252 | 66.694 | 1.00 21.68 | AAAA |
| ATOM | 2940 | CB | THR | 367 | 11.035 | 26.301 | 65.742 | 1.00 14.56 | AAAA |
| ATOM | 2941 | | THR | 367 | 10.085 | 26.545 | 64.697 | 1.00 21.76 | AAAA |
| | | | | | | | | 1.00 19.83 | |
| ATOM | 2942 | | THR | 367 | 12.340 | 25.825 | 65.138 | | AAAA |
| ATOM | 2943 | С | THR | 367 | 11.523 | 24.822 | 67.710 | 1.00 19.02 | AAAA |
| ATOM | . 2944 | 0 | THR | 367 | 12.071 | 23.717 | 67.625 | 1.00 21.79 | AAAA |
| ATOM | 2945 | N | LEU | 368 | 11.802 | 25.684 | 68.683 | 1.00 18.42 | AAAA |
| | | | | | | 25.348 | 69.700 | 1.00 21.02 | AAAA |
| ATOM | 2946 | CA | LEU | 368 | 12.797 | | | | |
| ATOM | 2947 | CB | LEU | 368 | 13.148 | 26.569 | 70.560 | 1.00 17.34 | AAAA |
| MOTA | 2948 | CG | LEU | 368 | 14.206 | 27.518 | 69.959 | 1.00 17.45 | AAAA |
| ATOM | 2949 | | LEU | 368 | 15.525 | 26.758 | 69.817 | 1.00 16.83 | AAAA |
| | | | | | | | 68.593 | 1.00 19.49 | AAAA |
| MOTA | 2950 | | LEU | 368 | 13.756 | 28.041 | | | |
| ATOM | 2951 | ن | LEU | 368 | 12.361 | 24.189 | 70.589 | 1.00 23.17 | AAAA |
| ATOM | 2952 | J | LEU | 368 | 13.203 | 23.420 | 71.052 | 1.00 24.81 | AAAA |
| ATOM | 2953 | N | GLU | 369 | 11.059 | 24.055 | 70.839 | 1.00 23.97 | AAAA |
| | | | | | | | 71.653 | 1.00 19.36 | AAAA |
| MOTA | 2954 | CA | GLU | 369 | 10.597 | 22.929 | | | |
| ATOM | 2955 | CB | GLU | 369 | 9.127 | 23.113 | 72.063 | 1.00 21.81 | Aaaa |
| ATOM | 2956 | CG | GLU | 369 | 8.913 | 24.225 | 73.100 | 1.00 40.15 | AAAA |
| ATOM | 2957 | CD | GLU | 369 | 7.450 | 24.416 | 73.487 | 1.00 49.38 | AAAA |
| | | | | | | | 73.905 | | AAAA |
| MOTA | 2958 | | GLU | 369 | 6.806 | 23.429 | | 1.00 43.26 | |
| ATOM | 2959 | OE2 | GLU | 369 | 6.948 | 25.558 | 73.382 | 1.00 57.31 | Aaaa |
| ATOM | 2960 | С | GLU | 369 | 10.778 | 21.623 | 70.859 | 1.00 24.29 | AAAA |
| | 2961 | 0 | GLU | 369 | 11.172 | 20.605 | 71.420 | 1.00 25.96 | AAAA |
| MOTA | | | | | | | 69.560 | 1.00 22.98 | AAAA |
| ATOM | 2962 | N | LYS | 370 | 10.488 | 21.643 | | | |
| MOTA | 2963 | CA | LYS | 370 | 10.665 | 20.437 | 68.746 | 1.00 23.19 | AAAA |
| MOTA | 2964 | CB . | LYS | 370 | 10.051 | 20.596 | 67.347 | 1.00 26.83 | AAAA |
| | | EG . | LYS | 370 | 8.537 | 20.461 | 67.287 | 1.00 36.68 | AAAA |
| ATOM | 2965 | | | | | | | | |
| MOTA | 2966 | CD | LYS | 370 | 8.056 | 20.431 | 65.832 | 1.00 39.85 | AAAA |
| ATOM | 2967 | CE | LYS | 370 | 6.567 | 20.105 | 65.740 | 1.00 56.23 | AAAA |
| ATCM · | 2968 | NZ | LYS | 370 | 6.082 | 19.996 | 64.326 | 1.00 56.10 | AAAA |
| | | | | 370 | 12.148 | 20.123 | 68.602 | 1.00 31.63 | AAAA |
| ATOM | 2969 | C | LYS | | | | | | |
| MOTA | 2970 | 0 | LYS | 370 | 12.549 | 18.958 | 68.587 | 1.00 36.88 | AAAA |
| · · · | | • | | | | | | • | • |

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| ATOM | 297 | '1 N | ALA | 371 | 12.9 | 61 21.17 | 0 68.493 | 1 1 00 | 26.25 | |
|----------|--------|-------|----------------------------------|-------------|--------|----------|----------|--------|-------|--------|
| ATOM | 297 | 2 CA | ALA | 371 | 14.40 | | | | | |
| MOTA | 297 | | | 371 | 15.0 | | | | 27.33 | AAAA |
| ATOM | 297 | | ALA | 371 | | | | | 23.70 | AAAA |
| ATOM | 297 | | ALA | | 14.98 | | | | 26.74 | AAAA |
| | 297 | | | 371 | 15.89 | | | | 29.52 | AAAA |
| ATOM | | | ALA | 372 | 14.48 | | , | | 24.83 | AAAA |
| MOTA | 297 | | | 372 | 14.95 | 59 20.05 | 72.012 | 1.00 | 34.24 | AAAA |
| MOTA | 297 | | ALA | 3 72 | 14.30 | 05 20.75 | | | 37.17 | AAAA |
| MOTA | 297 | 9 C | ALA | .372 | 14.66 | 3 18.564 | | | 45.62 | |
| MOTA | 298 | 0 0 | ALA | 372 | 15.56 | | | | | AAAA |
| ATOM | 298 | 1 N | ALA | 373 | 13.39 | | | | 35.52 | AAAA |
| MOTA | 298 | | ALA | 373 | 13.00 | | | | 44:50 | AAAA |
| ATOM | 298 | _ | ALA | 373 | | | | | 49.88 | AAAA |
| ATOM | 298 | | ALA | | 11.50 | | | | 49.32 | Aaaa |
| | | _ | | 373 | 13.80 | | | 1.00 | 44.64 | AAAA |
| ATOM | 298 | | ALA | 373 | 14.66 | | | | 58.19 | AAAA |
| ATOM | 298 | | ALA | 373 | 13.59 | 1 16.337 | 69.626 | | 41.63 | AAAA |
| HETATI | | | TAW | 1 | 36.36 | 8 43.907 | | | 13.03 | SOLV |
| HETATI | M 2981 | 3 OH2 | WAT: | 2 | 23.10 | 7 30.584 | | | 11.42 | |
| HETATI | 4 2989 | OH2 | WAT | 3 | 20.59 | | | | 14.73 | SOLV |
| HETATT | 1 2990 | OH2 | TAW | 4 | 31.35 | | | | | SOLV |
| HETATN | 1 2991 | | WAT | 5 | 30.38 | | | | 19.84 | SOLV |
| HETATN | | | TAW | 6 | 16.92 | | | 1.00 | 19.94 | SOLV |
| HETATM | | | WAT | 7 | | | | | 13.33 | SOLV |
| HETATM | | | WAT | | 28.44 | | | | 14.08 | SOLV |
| HETATM | | | | 8 | 40.37 | | | 1.00 | 19.10 | SOLV |
| | | | WAT | 9 | 18.45 | | | 1.00 | 18.81 | SOLV |
| HETATM | | | WAT | 10 | 26.30 | | | 1.00 | 16.65 | SOLV |
| HETATM | | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 11 | 50.14 | 5 32.063 | 58.142 | | 16.53 | SOLV |
| HETATM | | | WAT | 12 | 45.93 | 5 30.996 | 40.672 | | 25.08 | SOLV . |
| HETATM | | | WAT | 13 | 26.35 | 8 43.110 | 74.179 | | 22.91 | SOLV |
| HETATM | 3000 | OH2 | WAT | 14 | 48.727 | | 56.917 | | 25.49 | SOLV |
| HETATM | 3001 | OH2 | WAT | 15 | 30.244 | | 50.165 | | 25.78 | |
| HETATM | 3002 | OH2 | WAT | 16 | 10.615 | | 63.631 | | | SOLV |
| HETATM | 3003 | | WAT | 17 | 18.401 | | 62.704 | | 22.40 | SOLV |
| HETATM | | | WAT | 18 | 22.195 | | | | 21.46 | SOLV |
| HETATM | | | WAT | 19 | 3.278 | | 60.896 | | 26.19 | SOLV |
| HETATM | | | WAT | 20 | 23.643 | | 65.350 | | 20.38 | SOLV |
| HETATM | | | WAT | | | | 59.512 | | 21.27 | SOLV |
| HETATM | | OH2 | | 21 | 50.287 | | 48.818 | 1.00 | | SOLV |
| HETATM | | | | 22 | 44.725 | | 46.541 | 1.00 | | SOLV |
| HETATM | | OH2 | | 23 | 8.346 | | 49.922 | 1.00 | | SOLV |
| | | OH2 | | 24 | 39.855 | | 67.390 | 1.00 | 20.43 | SOLV |
| HETATM | | OH2 | | 25 | 7.827 | | 57.779 | 1.00 | 19.24 | SOLV |
| HETATM | | OH2 | | 26 | 45.388 | | 36.246 | 1.00 | 20.86 | SOLV |
| HETATM | | OH2 | | 27 | 47.636 | | 33.388 | 1.00 | 20.41 | SOLV |
| HETATM | | OH2 | | 28 | 32.514 | 35.684 | 41.278 | 1.00 | 24.76 | SOLV |
| HETATM | | OH2 | | 29 | 26.188 | 15.341 | 61.913 | 1.00 | | SOLV |
| HETATM | 3016 | OH2 | WAT | 30 | 14.957 | 43.169 | 56.333 | 1.00 | | SOLV |
| HETATM | 3017 | OH2 | WAT | 31 | 24.483 | 43.556 | 55.704 | 1.00 | | SOLV |
| HETATM | 3018 | OH2 | WAT | 3 2 | 41.141 | | 48.456 | 1.00 | | SOLV |
| HETATM | 3019 | OH2 | WAT | 33 | 23.104 | | 54.086 | 1.00 | | |
| HETATM | 3020 | OH2 | | 34 | 51.301 | 28.602 | 57.694 | 1.00 | | SOLV |
| HETATM | | OH2 | | 35 | 51.376 | 29.469 | 53.156 | | | SOLV |
| HETATM | | OH2 | | 36 | 12.518 | 22.131 | | | | SOLV |
| HETATM | | OH2 | | | 6.521 | 22.131 | 49.816 | 1.00 | | SOLV |
| HETATM | | | | 37 | | 27.442 | 50.861 | 1.00 2 | | SOLV |
| | | ОН2 ; | | 38 | 30.390 | 33.757 | 34.190 | 1.00 | L9.87 | SOLV |
| HETATM | | OH2 | | 39 | 8.328 | 29.586 | 62.062 | 1.00 3 | 32.01 | SOLV |
| HETATM | | OH2 V | | 40 | 30.180 | 24.235 | 30.724 | 1.00 2 | 22.61 | SOLV |
| HETATM | | OH2 V | | 41 | 44.521 | 30.663 | 38.395 | 1.00 2 | | SOLV |
| HETATM | | OH2 V | <i>I</i> AT | 42 | 30.981 | 18.043 | 41.186 | 1.00 2 | | SOLV |
| HETATM | | OH2 V | TAI | 43 | 14.632 | 37.127 | 73.830 | 1.00 2 | | SOLV |
| HETATM | 3030 | OH2 W | JAT | 44 | 39.332 | 25.953 | 72.230 | 1.00 2 | | SOLV |
| HETATM . | 3031 | OH2 W | | 45 | 7.597 | 37.592 | 51.896 | 1.00 3 | | SOLV |
| HETATM | | OH2 W | | 46 | 15.027 | 18.079 | 54.827 | 1.00 2 | | |
| HETATM | | OH2 W | TAT | 47 | 11.076 | 45.493 | 66.435 | | | SOLV |
| HETATM | | OH2 W | | 48 | 42.124 | 18.055 | | 1.00 3 | | SOLV |
| ETATM | | OH2 W | | 49 | 48.736 | 25.764 | 37.233 | 1.00 2 | | SOLV |
| ETATM | | | | | | | 64.149 | 1.00 3 | | SOLV |
| ETAIM . | | OH2 W | AT' | 50 | 50.383 | 27.254 | 54.972 | 1.00 2 | 4.36 | SOLV |

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| HETATN | 4 3037 | CH | 2 WAT | 51 | 48.659 | 36.025 | 68.226 | 1.00 33.89 | SOLV |
|--------|--------|------|-------|-------------|-----------------|---------|-----------------|------------|--------|
| HETATN | | | 2 WAT | | | | | | |
| | | | | | 36.998 | | | 1.00 21.03 | SOLV |
| HETATN | 13039 | OH | 2 WAT | 53 | 41.303 | 16.309 | 55.307 | 1.00 32.23 | SOLV |
| HETAT | 1 3040 | OH | 2 WAT | 54 | 33,242 | 39.524 | 49.454 | 1.00 29.77 | |
| | _ | | | | | | | | SOLV |
| HETATN | 1 3041 | OH | 2 WAT | 55 | 45.004 | 25.973 | 35.031 | 1.00 21.59 | SOLV |
| HETATM | 1 3042 | OH | 2 WAT | 56 | 19.039 | 25.829 | 45.793 | 1.00 33.48 | SOLV |
| | | | | | | | | | |
| HETATM | | | 2 WAT | 5 7 | 17.922 | 35.542 | 50.154 | 1.00 37.51 | SOLV |
| HETATM | 1 3044 | OH | 2 WAT | 58 | 10.409 | 26.864 | 73.166 | 1.00 26.54 | SOLV |
| HETATM | | | 2 WAT | 59 | 11.835 | 22.805 | 59.408 | | |
| | | | | | | | | 1.00 20.83 | SOLV |
| HETATM | 3046 | OH | 2 WAT | 60 . | 18.254 | 48.699 | 53.224 | 1.00 28.41 | . SOLV |
| HETATM | 3047 | OH | Z WAT | 61 | 10.426 | 26.647 | 60.447 | 1.00 32.72 | SOLV |
| | _ | _ | | | | | | | |
| HETATM | | | Z WAT | 62 | 21.304 | 55.086 | 63.510 | 1.00 28.84 | SOLV |
| HETATM | 13049 | OH | TAW S | 63 | 32.532 | 51.211 | 45.469 | 1.00 32.48 | SOLV |
| HETATM | 3050 | OH' | Z WAT | 64 | 22.658 | 61.079 | 57.420 | 1.00 27.32 | • |
| | | | | | | | | | SOLV |
| HETATM | 3051 | OH | YAW S | 65 | 16.734 | 24.334 | 74.721 | 1.00 27.44 | SOLV |
| HETATM | 3052 | OH | TAW S | 66 | 32.758 | 37.824 | 54.391 | 1.00 25.07 | SOLV |
| | | | | | | | | | |
| HETATM | | | TAW S | 67 | 11.142 | 25.859 | 49.706 | 1.00 29.66 | SOLV |
| HETATM | 3054 | OH2 | TAW S | 68 | 24.192 | 15.261 | 53.236 | 1.00 30.21 | SOLV |
| HETATM | 3055 | OHO | TAW S | 69 | 19.816 | 17.916 | 66.357 | 1.00 30.50 | |
| | | | | | | | | | SOLV |
| HETATM | 3056 | OH2 | TAW S | 70 | 5 0. 347 | 23.975 | 53.197 | 1.00 28.08 | SOLV |
| HETATM | 3057 | OH2 | MAT | 71 | 50.258 | 30.918 | 51.113 | 1.00 20.19 | SOLV |
| | | | | | | | | | |
| HETATM | | | TAW ? | 72 | 21.047 | 17.624 | 68.693 | 1.00 41.23 | SOLV |
| HETATM | 3059 | OHZ | WAT | 73 | 26.782 | 33.756 | 49.995 | 1.00 25.80 | SOLV |
| HETATM | 3060 | OH 2 | TAW | 74 | 12.570 | 43.844 | 64.441 | 1.00 31.03 | SOLV |
| | | | | | | | | | |
| HETATM | 3001 | OHZ | TAW | 75 | 35.555 | 41.287 | 50.852 | 1.00 24.03 | SOLV |
| HETATM | 3062 | OH2 | TAW | 76 | 27.764 | 18.231 | 61.827 | 1.00 18.28 | SOLV |
| HETATM | | | WAT | 7 7 | 26.715 | 29.236 | 38.391 | 1.00 23.18 | |
| | | | | | | | | | SOLV |
| HETATM | 3064 | OH2 | WAT | 78 | 21.461 | 23.245 | 48.872 | 1.00 23.80 | SOLV |
| HETATM | 3065 | OH2 | WAT | 79 | 49.246 | 28.263 | 65.477 | 1.00 21.52 | SOLV |
| | | | | | | | | | |
| HETATM | _ | | WAT | 80 | 31.785 | 13.301 | 69.606 | 1.00 31.11 | SOLV |
| HETATM | 3067 | OH2 | WAT | 81 | 49.811 | 34.740 | 59.229 | 1.00 31.76 | SOLV |
| HETATM | 3068 | OH2 | WAT | 82 | 45.670 | 33.188 | 42.470 | 1.00 23.13 | SOLV |
| | | | | | | | | | |
| HETATM | 3069 | | WAT | 83 | 9.408 | 39.751 | 55.872 | 1.00 31.53 | SOLV |
| HETATM | 3070 | OH2 | WAT | 84 - | 35.166 | 35.2878 | 29.899 | 1.00 37.32 | SOLV |
| HETATM | 3071 | OH2 | WAT | 85 | 41.927 | 22.970 | 73.694 | 1.00 44.07 | SOLV |
| | | | - | | | | | • | |
| HETATM | 3072 | OHZ | WAT | 86 | 22.125 | 34.577 | 49.199 | 1.00 44.65 | SOLV |
| HETATM | 3073 | OH2 | WAT | 87 | 43.984 | 33.541 | 37.965 | 1.00 24.88 | SOLV |
| HETATM | | | WAT | 88 | 11.997 | 17.962 | 56.312 | 1.00 34.85 | |
| | | | | | | | | | SOLV |
| HETATM | 3075 | OH2 | WAT | 89 | 42.194 | 14.737 | 59.766 | 1.00 25.91 | SOLV |
| HETATM | 3076 | OH2 | WAT | 90 | 49.313 | 24.200 | 41.684 | 1.00 29.29 | SOLV |
| | | | WAT | 91 | 48.504 | 33.595 | 61.519 | | |
| HETATM | | | | | | | | 1.00 30.32 | SOLV |
| HETATM | 3078 | OH2 | VAT | 92 | 24.773 | 18.356 | 33.365 | 1.00 53.13 | SOLV |
| HETATM | 3079 | OH2 | WAT | 93 | 35.160 | 35.656 | 47.470 | 1.00 41.41 | SOLV |
| | | | | | 44.682 | 36.658 | | | |
| HETATM | | | WAT | 94 | | | 39.962 | 1.00 29.24 | SOLV |
| HETATM | 3081 | OH2 | WAT | 95 | . 9.576 | 41.033 | 52.549 | 1.00 51.83 | · SOLV |
| HETATM | 3082 | OH2 | WAT | ^6 | 47.199 | 20.112 | 42.102 | 1.00 40.39 | SOLV |
| | - | | | | 49.254 | 26.331 | | | |
| HETATM | | | WAT | 7ر ٠ | | - | 59.641 | 1.00 37.03 | SOLV |
| HETATM | 3084 | OH2 | TAW | -8 | 26.808 | 37.600 | 38.172 | 1.00 28.74 | SOLV |
| HETATM | 3085 | OH2 | WAT | 99 | 40.749 | 14.572 | 64.635 | 1.00.33.42 | SOLV |
| | | | | | | - | | | |
| HETATM | 3086 | | WAT | 100 | 24.850 | 44.161 | 47.775 | 1.00 27.89 | SOLV |
| HETATM | 3087 | OH2 | WAT | 101 | 34.326 | 42.063 | 46.714 | 1.00 42.22 | SOLV |
| HETATM | | | WAT | 102 | 30.226 | 34.544 | 52.026 | 1.00 30.77 | |
| | | | | | | | | | SOLV |
| HETATM | 3089 | OH2 | WAT | 103 | 47.824 | 39.054 | 78.09 7 | 1.00 52.16 | SOLV |
| HETATM | 3090 | OH2 | WAT | 104 | 19.665 | 18.953 | 47.438 | 1.00 51.70 | SOLV |
| | | | | | 46.857 | | | | |
| HETATM | | OH2 | | 105 | | 36.525 | 46.232 | 1.00 23.65 | SOLV |
| HETATM | 3092 | OH2 | WAT | 106 | 48.069 | 19.460 | 67.360 | 1.00 37.56 | SOLV |
| HETATM | | OH2 | WAT | 107 | 15.553 | 56.850 | 61.838 | 1.00 46.95 | SOLV |
| | | | | | | | | | |
| HETATM | 3094 | OH2 | | 108 | 44.026 | 19.119 | 70.671 | 1.00 39.55 | SOLV |
| HETATM | 3095 | OH2 | WAT | 109 | 8.139 | 42.064 | 65.674 | 1.00 42.61 | SOLV |
| HETATM | | OH2 | | 110 | 50.624 | 36.591 | 65.779 | 1.00 31.59 | SOLV |
| | | | | | | | | | |
| HETATM | 3097 | OH2 | WAT | 111 | 51.398 | 26.073 | 61.043 | 1.00 49.09 | SOLV |
| HETATM | | OH2 | WAT | 112 | 26.174 | 33.692 | 33.551 | 1.00 36.61 | SOLV |
| | | | | | 23.545 | | | 1.00 24.34 | |
| HETATM | | OH2 | | 113 | | 20.203 | 53.001 | | SOLV |
| HETATM | 3100 | OH2 | TAW | 114 | 9.083 | 42.965 | 5 7 .697 | 1.00 33.65 | SOLV |
| HETATM | | OH2 | | 115 | 8.442 | 39.898 | 64.594 | 1.00 31.21 | SOLV |
| | | | | | | | | | |
| HETATM | 102د | OH2 | WAT | 116 . | 15.219 | 35.897 | 51.951 | 1.00 26.59 | SOLV |

| HETAT | M 310 | 3 OH | 2 WAT | 117 | | 15.41 | 7 38. | 438 | 50.473 | 1.0 | 0 34.46 | | SOLV |
|----------------------|--------|-------|------------|------------|-----|------------------|----------------|--------|------------------|-------|----------------|----|--------------|
| HETAT: | M 310 | 4 OH | 2 WAT | 118 | | 40.75 | | | 29.206 | | 0 29.12 | | SOLV |
| HETAT | M 310 | 5 OH | 2 WAT | 119 | | 27.71 | 7 18. | 542 | 46.553 | | 0 28.17 | | SOLV |
| HETAT | M 310 | 6 OH. | 2 WAT | 120 | | 18.61 | 2 13. | 786 | 56.845 | | 0 38.56 | | SOLV |
| HETAT | M 310 | 7 OH: | 2 WAT | 121 | | 43.198 | 3 31. | 377 | 72.139 | | 0 26.31 | | SOLV |
| HETAT | M 310 | 8 OH: | 2 WAT | 122 | | 44.188 | | | 33.802 | | 0 29.81 | | SOLV |
| HETAT | M 3109 | | 2 WAT | | | 50.736 | | | 58.456 | | 0 32.40 | | SOLV |
| HETATI | M 311(| | 2 WAT | | | 31.302 | | | 31.742 | | 0 30.84 | | SOLV |
| HETATI | M 311 | 1 OH2 | 2 WAT | 125 | | 36.895 | | | 34.198 | | 0 34.67 | | SOLV |
| HETATI | M 3112 | 2 OH2 | TAW S | | | 47.474 | | | 67.427 | | 0 34.35 | | SOLV |
| HETATI | M 3113 | 3 OH2 | TAW S | 127 | | 7.178 | | | 64.063 | | 31.77 | | SOLV |
| HETATI | 4 3114 | 1 OH2 | TAW S | 128 | | 36.362 | | | 54.021 | | 36.88 | | SOLV |
| HETATI | M 3115 | OH2 | TAW S | 129 | | 42.486 | 35.5 | 503 | 30.348 | | 26.61 | | SOLV |
| HETATI | 4 3116 | 5 OH2 | TAW S | 130 | | 8.432 | 34.3 | 383 | 50.442 | | 37.45 | | SOLV |
| HETATI | 4 3117 | 7 OH2 | TAW S | 131 | | 37.644 | 49.0 | 018 | 48.946 | | 37.33 | | SOLV |
| HETATI | 4 3118 | 3 OH2 | WAT. | 132 | • | 50.273 | 41.6 | 545 | 63.380 | | 37.33 | | SOLV |
| HETAT | 1 3119 | OH2 | YAW ? | 133 | | 7.518 | 26.6 | 533 | 61.571 | | 45.42 | | SOLV |
| HETATA | 4 3120 |) OH2 | TAW | 134 | | 31.483 | 46.1 | L97 | 72.538 | | 28.02 | | SOLV |
| HETATN | 1 3121 | . OH2 | TAW | 135 | | 41.501 | 16.6 | 504 | 58.054 | 1.00 | 32.78 | | SOLV |
| HETATA | 1 3122 | OH2 | TAW | 136 | | 45.898 | 47.7 | | 55.185 | 1.00 | 43.47 | | SOLV |
| HETATI | 1 3123 | | WAT | 137 | | 16.300 | | 514 | 49.519 | | 30.37 | | SOLV |
| HETATM | 1 3124 | | WAT | 138 | | 51.148 | 36.9 | | 55.148 | | 46.34 | | SOLV |
| HETATM | 1 3125 | | WAT | 139 | | 21.525 | 53.7 | 61 | 50.892 | | 38.27 | | SOLV |
| HETATM | 1 3126 | OH2 | WAT | 140 | | 21.603 | 54.5 | 088 | 68.690 | 1.00 | 33.10 | | SOLV |
| HETATM | | | WAT | 141 | | 10.191 | | | 60.325 | | 30.24 | | SOLV |
| HETATM | | | WAT | 142 | | 16.951 | | .20 | 66.901 | | 40.85 | | SOLV |
| HETATM | | | WAT | 143 | | 4.943 | | | 51.199 | 1.00 | 49.13 | | SOLV |
| HETATM | | | WAT | 144 | | 10.711 | | | 58.177 | 1.00 | 30.72 | | SOLV |
| HETATM | | | WAT | 145 | | 30.815 | | | 36.040 | 1.00 | 42.23 | | SOLV |
| HETATM | | | WAT | 146 | | 21.763 | 24.5 | | 46.695 | | 28.31 | | SOLV |
| HETATM | | | WAT . | | | 51.788 | | | 50.887 | | 26.15 | | SOLV |
| HETATM | | | WAT | 148 | | 24.531 | 44.7 | | 72.420 | | 27.99 | | SOLV |
| HETATM | | | TAW | 149 | | 50.938 | 23.4 | | 60.422 | | 38.20 | | SOLV |
| HETATM HETATM | | - | TAW TAW | 150 | | 24.860 | 47.9 | | 61.067 | | 18.89 | | SOLV |
| HETATM | | | WAT | 151 152 | | 27.336 38.680 | 37.3 | | 35.642 | | 33.58 | | SOLV |
| HETATM | | | WAT | 153 | | 24.441 | 35.5 16.0 | | 35.974 | | 26.89 | | SOLV |
| HETATM | | | WAT | 154 | | 20.343 | 18.1 | | 33.317 73.416 | | 48.33 | | SOLV |
| HETATM | | OH2 | | 155 | | 49.765 | 37.9 | | 74.801 | | 36.28 | | SOLV |
| HETATM | | OH2 | | 156 | | 34.329 | 31.1 | | 47.547 | | 48.41 25.33 | | SOLV |
| HETATM | | OH2 | | 157 | | 43.028 | 24.5 | | 72.536 | | 41.54 | | SOLV SOLV |
| HETATM | | OH2 | | 158 | | 39.888 | 15.0 | | 42.035 | | 28.76 | | SOLV |
| HETATM | | OH2 | | 159 | | 41.886 | 20.7 | | 73.179 | | 51.03 | | SOLV |
| HETATM | 3146 | OH2 | WAT | 160 | | 22.962 | 49.9 | | 58.518 | | 35.04 | | SOLV |
| HETATM | 3147 | OH2 | WAT | 161 | | 14.696 | 15.20 | | 68.016 | | 55.47 | | SOLV |
| HETATM | 3148 | OH2 | WAT | 162 | | 14.915 | 18.18 | | 64.866 | | 42.00 | | SOLV |
| HETATM | 3149 | OH2 | WAT | 163 | | 30.608 | 49.02 | | 52.612 | | 47.32 | | SOLV |
| HETATM | 3150 | OH2 | WAT | 164 | 5 | 52.566 | 30.90 | 06 | 57.612 | | 36.71 | | SOLV |
| HETATM | - | OH2 | | 165 | 2 | 23.699 | 27.33 | 31 | 77.729 | | 32.22 | | SOLV |
| HETATM | | ОН2 | | 166 | 3 | 36.971 | 59.04 | 16 | 63.272 | 1.00 | 43.05 | | SOLV |
| HETATM | | OH2 | | 167 | | 16.053 | | 27 | 52.876 | 1.00 | 33.66 | : | SOLV |
| HETATM | | OH2 | | 168 | | 12.780 | 49.15 | 51 | 58.106 | .1.00 | | | SOLV |
| HETATM | | OH2 | | 169 | | 15.100 | 44.50 | | 72.183 | 1.00 | 45.43 | : | SOLV |
| HETATM | | OH2 | | 170 | | 1.677 | 60.99 | | 50.050 | 1.00 | 34.51 | : | SOLV |
| HETATM | | OH2 | | 171 | | 5.336 | 45.67 | | 45.578 | 1.00 | 55.85 | | SOLV |
| HETATM | | OH2 | | 172 | | 7.481 | 18.26 | | 49.018 | 1.00 | 32.73 | 5 | OLV |
| HETATM | | OH2 | | 173 | | 6.112 | 18.14 | - | 31.404 | | 49.94 | | OLV |
| HETATM | | OH2 | | 174 . | | 5.874 | 43.14 | | 70.985 | | 32.89 | | SOLV |
| HETATM | | OH2 V | | 175 | | 4.517 | 17.88 | - | 33.278 | | 42.20 | | OLV |
| HETATM | | OH2 | | 176 | | 6.330 | 54.88 | | 50.466 | | 40.74 | | OLV |
| HETATM | | OH2 | | 177 | | 1.400 | 51.08 | | 74.689 | | 38.56 | | OLV |
| HETATM | | OH2 V | | 178 | | 0.971 | 27.07 | | 57.130 | | 44.49 | | OLV |
| HETATM | | OH2 V | | 179 | | 7.933 | 23.41 | _ | 54.691 | | 42.84 | | OLV |
| HETATM | | OH2 V | | 180 | | 3.498 | 47.59 | | 73.612 | | 35.99 | | OLV |
| HETATM : HETATM : | | OH2 V | | 181 | | 6.016 | 19.58 17.02 | - • | 14.954 | | 51.31 | | OLV |
| aciain. | 100 | OH2 W | 1327 | 182 | . 4 | 0.139 | 17.02 | . 0 _7 | 74.920 | 1.00 | 43.64 | ٤. | OLV |

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| HETATM 3169 | OH2 WAT | 183 | 10.441 | 42.659 | 62.744 | 1.00 34.51 | SOLV |
|--------------------|-----------|-----|----------|------------------|------------------|------------|------|
| HETATM 3170 | | 184 | 2.095 | 34.482 | 65.810 | 1.00 36.49 | SOLV |
| HETATM 3171 | L OH2 WAT | 185 | 45.749 | 18.286 | 51.615 | 1.00 28.19 | SOLV |
| HETATM 3172 | | 186 | 25.771 | 38.332 | 76.707 | 1.00 45.53 | SOLV |
| HETATM 3173 | | 187 | 7.228 | 40.382 | 57.542 | 1.00 48.91 | SOLV |
| HETATM 3174 | OH2 WAT | 188 | 42.972 | 52.824 | 67.739 | 1.00 39.99 | SOLV |
| HETATM 3175 | | 189 | 20.137 | 13.189 | 73.277 | 1.00 44.91 | SOLV |
| HETATM 317- | | 190 | 48.945 | 19.193 | 47.581 | 1.00 52.88 | SOLV |
| HETATM 3176 | | 191 | 14.549 | 34.547 | 47.665 | 1.00 49.15 | SOLV |
| HETATM 3177 | | 192 | 31.765 | 20.567 | 26.536 | 1.00 42.23 | SOLV |
| HETATM 3178 | | 193 | 9.784 | 39.303 | 74.222 | 1.00 32.10 | SOLV |
| HETATM 3179 | | 194 | 28.865 | 12.481 | 52.375 | 1.00 50.98 | SOLV |
| HETATM 3180 | | 195 | - 24.030 | 12.804 | 70.409- | 1.00 52.43 | SOLV |
| нетати 3181 | | 196 | 47.209 | 39.536 | 50.698 | 1.00 43.03 | SOLV |
| HETATM 3182 | OH2 WAT | 197 | 35.618 | 18.114 | 27.306 | 1.00 41.11 | SOLV |
| HETATM 3183 | OH2 WAT | | 23.625 | 48.145 | 43.853 | 1.00 48.20 | SOLV |
| HETATM 3184 | OH2 WAT | 198 | 37.090 | 59.044 | 54.185 | 1.00 34.99 | SOLV |
| HETATM 3185 | OH2 WAT | 199 | | 12.208 | 59.080 | 1.00 36.58 | SOLV |
| HETATM 3186 | OH2 WAT | 200 | 34.478 | 29.583 | 76.228 | 1.00 33.95 | SOLV |
| HETATM 3187 | | 201 | 22.142 | 42.619 | 53.973 | 1.00 40.44 | SOLV |
| HETATM 3188 | OH2 WAT | 202 | 13.608 | 18.701 | 72.526 | 1.00 55.64 | SOLV |
| HETATM 3189 | OH2 WAT | 203 | 42.647 | | 77.480 | 1.00 33.04 | SOLV |
| HETATM 3190 | OH2 WAT | 204 | 37.005 | 35.993 | | 1.00 34.82 | SOLV |
| HETATM 3191 | OH2 WAT | 205 | 34.154 | 20.512 | 33.327 47.642 | 1.00 31.00 | SOLV |
| HETATM 3192 | OH2 WAT | 206 | 37.264 | 57.546 | - | 1.00 49.36 | SOLV |
| HETATM 3193 | OH2 WAT | 207 | 17.924 | 35.195 | 79.003 62.378 | 1.00 35.43 | SOLV |
| HETATM 3194 | OH2 WAT | 208 | 51.172 | 31.581 | 79.224 | 1.00 39.95 | SOLV |
| HETATM 3195 | OH2 WAT | 209 | 50.503 | 36.726 | 63.852 | 1.00 52.08 | SOLV |
| HETATM 3196 | OH2 WAT | 210 | 18.382 | 13.162 8.351 | 55.199 | 1.00 32.00 | SOLV |
| HETATM 3197 | OH2 WAT | 211 | 27.245 | | 59.540 | 1.00 39.12 | SOLV |
| HETATM 3198 | OH2 WAT | 212 | 18.354 | 13.545 51.744 | 63.388 | 1.00 36.69 | SOLV |
| HETATM 3199 | OH2 WAT | 213 | 49.088 | | 50.871 | 1.00 38.03 | SOLV |
| HETATM 3200 | OH2 WAT | 214 | 23.251 | 33.160 35.073 | 50.651 | 1.00 38.63 | SOLV |
| HETATM 3201 | OH2 WAT | 215 | 12.989 | | 43.239 | 1.00 37.93 | SOLV |
| HETATM 3202 | OH2 WAT | 216 | 24.414 | 44.460 | 73.117 | 1.00 34.17 | SOLV |
| HETATM 3203 | OH2 WAT | 217 | 24.690 | 47.590 17.949 | 81.360 | 1.00 40.74 | SOLV |
| HETATM 3204 | OH2 WAT | 218 | 19.844 | | 74.247 | 1.00 37.83 | SOLV |
| HETATM 3205 | | 219 | 40.169 | 27.215 39.516 | 73.171 | 1.00 49.20 | SOLV |
| HETATM 3206 | | 220 | 38.737 | | 46.879 | 1.00 45.57 | SOLV |
| HETATM 3207 | OH2 WAT | 221 | 50.628 | 21.408 | 75.660 | 1.00 37.33 | SOLV |
| HETATM 3208 | OH2 WAT | 222 | 35.436 | 43.288 | 55.285 | 1.00 37.33 | SOLV |
| HETATM 3209 | OH2 WAT | 223 | 34.390 | 16.963 | 34.475 | 1.00 46.29 | SOLV |
| HETATM 3210 | OH2 WAT | 224 | 21.800 | 35.454 | 46.787 | 1.00 40.23 | SOLV |
| HETATM 3211 | OH2 WAT | 225 | 15.751 | 40.989 | 66.295 | 1.00 38.35 | SOLV |
| HETATM 3212 | OH2 WAT | 226 | 23.844 | 48.662 | 55.117 | 1.00 38.33 | SOLV |
| HETATM 3213 | OH2 WAT | 227 | 47.225 | 20.562 | | 1.00 49.99 | SOLV |
| #FTATM 3214 | | 228 | 23.426 | 19.272 | 50.565 | 1.00 30.07 | 2070 |

| | | | | | | n v | • • | ~ | 000 | | | |
|--------------|----------|--------|------------|----|---------|------------------|------------------|------------------|--------|-------|---------|----|
| ATOM | 1 | СВ | ALA | λ | Residue | | Y 36 963 | Z 25 052 | OCC. | B | Segment | ID |
| | 2 | | ALA | | 2 | 43.739 | 36.862 | 75.052 | | 64.01 | 6 | |
| MOTA | | | ALA | | | 44.405 | 38.106 | 72.971 | | 60.02 | 6 | |
| ATOM | 3 4 | И | ALA | | - | 43.251 | 38.536 | 72.908 | | 57.94 | 8 | |
| ATOM | 5 | | ALA | | 2 | 46.142 | 37.179 | 74.497 | | 62.88 | 7 | |
| MOTA | | CA | LYS | | 2 | 44.776 | 36.966 | 73.923 | | 63.02 | 6 | |
| MOTA | 6 7 | N · | | | 3 | 45.398 | 38.588 | 72.233 | | 55.40 | 7 | |
| ATOM | | CA | LYS | | 3 | 45.196 | 39.671 | 71.287 | | 53.02 | 6 | |
| ATOM | 8 | CB | LYS | | 3 | 46.443 | 39.830 | 70.421 | | 53.11 | 6 | |
| ATOM | 9 | CG | LYS | | | 47.703 | 40.093 | 71.217 | | 57.36 | 6 | |
| ATOM | 10 | CD | LYS | | 3 | 48.941 | 39.976 | 70.349 | | 60.94 | 6 | |
| ATOM | 11 | CE | LYS | | 3 | 48.909 | 40.957 | 69.196 | | 63.48 | 6 | |
| ATOM | 12 | NZ | LYS | | 3 | 50.075 | 40.765 | 68.294 | | 66.87 | 7 | |
| ATOM | 13 | C | LYS | | 3 | 43.986 | 39.401 | 70.399 | | 50.49 | 6 | |
| MOTA | 14 | 0 | LYS | | 3 | 43.691 | 38.255 | 70.063 | | 52.50 | 8 | |
| ATOM | 15 | N | VAL | | 4 | 43.281 | 40.464 | 70.034 | | 45.96 | 7 | |
| ATOM | 16 | CA | VAL | | 4 | 42.122 | 40.352 | 69.167 | | 41.16 | 6 | |
| ATOM | 17 | CB | VAL | | 4 | 40.983 | 41.272 | 69.638 | | 41.53 | 6 | |
| ATOM | 18 | | VAL | | 4 | 39.734 | 41.028 | 68.797 | | 40.07 | 6 | |
| ATOM | 19 | | VAL | | 4 | 40.705 | 41.033 | 71.115 | | 38.31 | 6 | |
| MOTA | 20 | C | VAL | | 4 | 42.619 | 40.796 | 67.796 | | 39.96 | 6 | |
| ATOM. | 21 | 0 | VAL | | 4 | 43.123 | 41.914 | 67.645 | 1.00 | | 8 | |
| MOTA | 22 | N | LYS | | 5 | 42.486 | 39.916 | 66.807 | | 36.24 | 7 | |
| MOTA | 23 | CA | LYS | | 5 | 42.956 | 40.186 | 65.449 | 1.00 | | 6 . | |
| ATOM | 24 | CB | LYS | | 5 | 43.930 | 39.088 | 65.024 | 1.00 | | 6 | |
| MOTA | 25 | CG | LYS | | 5 | 45.197 | 38.978 | 65.860 | 1.00 | | 6 | |
| MOTA | 26 | CD | LYS | | 5 | 46.113 | 40.179 | 65.659 | 1.00 | | 6 | |
| MOTA | 27 28 | CE | LYS | | 5 5 | 47.436 | 39.957 | 66.369 | 1.00 | | 6 | |
| MOTA | 29 | NZ | LYS LYS | | 5 | 48.345 | 41.121 40.254 | 66.245 | 1.00 | | 7 | |
| ATOM ATOM | 30 | С 0 | LYS | | 5 | 41.840 40.788 | 39.641 | 64.415 | 1.00 | | 6 | |
| MOTA | 31 | N | LEU | | 6 | 42.082 | 40.983 | 64.588 63.329 | 1.00 | | 8 | |
| ATOM | 32 | CA | LEU | | 6 | 41.097 | 41.094 | 62.253 | 1.00 | | 7 6 | |
| ATOM | 33 | CB | LEU | | 6 | 40.589 | 42.532 | 62.114 | 1.00 | | 6 | |
| MOTA | 34 | CG | LEU | | 6 | 39.346 | 42.823 | 61.248 | 1.00 | | 6 | |
| ATOM | 35 | | LEU | | 6 | 39.356 | 44.295 | 60.899 | 1.00 | | 6 | |
| ATOM | 36 | | LEU | | 6 | 39.336 | 42.031 | 59.964 | | 32.87 | | |
| ATOM | 37 | c | LEU | | 6 | 41.802 | 40.721 | 60.955 | 1.00 | | 6 | |
| ATOM | 38 | ō | LEU | | 6 | 42.631 | 41.491 | 60.468 | 1.00 | | 8 | |
| MOTA | 39 | N | ILE | | 7 | 41.494 | 39.561 | 60.382 | 1.00 | | 7 | |
| ATOM | 40 | CA | ILE . | | 7 | 42.145 | 39.199 | 59.129 | 1.00 | | 6 | |
| ATOM | 41 | CB | ILE . | | 7 | 42.062 | 37.711 | | 1.00 | | 6 | |
| ATOM | 42 | CG2 | ILE | | 7 | 42.731 | 37.409 | 57.517 | 1.00 | | 6. | |
| ATOM | 43 | | ILE | | 7 | 42.746 | 36.941 | 59.975 | 1.00 | | 6 | |
| ATOM | 44 | | ILE . | | 7 | 42.744 | 35.451 | 59.755 | 1.00 | | 6 | |
| ATOM | 45 | C | ILE A | Ą | 7 | 41.487 | 39.935 | 57.971 | 1.00 | | 6 | |
| ATOM | 46 | 0 | ILE A | | 7 | 40.258 | 39.933 | 57.855 | 1.00 | | 8 | |
| MOTA | 47 | N | GLY A | A | 8 | 42.304 | 40.563 | 57.124 | 1.00 | 37.25 | . 7 | |
| ATOM " | 48 | CA | GLY A | A | 8 | 41.771 | 41.305 | 55.994 | 1.00 | 38.69 | 6 | |
| MOTA | 49 | С | GLY A | Ą | 8 | 42.809 | 41.939 | 55.079 | 1.00 | | 6 | |
| ATOM | 50 | 0 | GLY A | A | 8 | 44.015 | 41.827 | 55.321 | 1.00 | 39.21 | 8 | |
| ATOM | 51 | N | THR A | £. | 9 | 42.335 | 42.622 | 54.033 | 1.00 | 39.41 | 7 | |
| ATOM | 52 | CA | THR A | A. | 9 | 43,.212 | 43.268 | 53.057 | 1.00 | 38.69 | 6 . | |
| ATOM | 53 | CB | THR A | 1 | 9 | 44.132 | 42.210 | 52.390 | 1.00 | 37.27 | 6 | |
| ATOM | 54 | OG1 | THR 2 | A. | 9 | 44.754 | 42.771 | 51.230 | 1.00 | 36.82 | 8 | |
| MOTA | 55 | CG2 | THR A | 1 | 9 | 43.332 | 40.972 | 52.001 | 1.00 | 38.59 | 6 | |
| ATOM | 56 | Ç | THR A | 1 | 9 | 42.447 | 44.045 | 51.970 | 1.00 | 38.60 | 6 | |
| ATOM | 57 | 0 | THR P | Ŧ | 9 | 41.434 | 43.569 | 51.452 | 1.00 | 37.30 | 8 | |
| ATOM | 58 | 14 | LEU A | | 10 | 42.939 | 45.238 | 51.628 | 1.00 | | 7 | |
| MOTA | 59 | | LEU A | | 10 | 42.304 | 46.077 | 50.609 | 1.00 | 39.39 | 6 | |
| ATOM | 60 | CB | LEU A | | 10 | 43.026 | 47.418 | 50.456 | 1.00 3 | 38.98 | 6 | |
| ATOM | 61 | CG | LEU A | | 10 | 42.836 | 48.506 | 51.510 | 1.00 3 | 39.68 | 6 | |
| ATOM | 62 | | LEU A | | 10 | 41.343 | 48.830 | 51.594 | 1.00 4 | | 6 | |
| MOTA | 63 | CD2 | LEU A | | 10 | 43.382 | 48.057 | 52.857 | 1.00 4 | | 6 | |
| ATOM | ć÷ | С | LEU A | | 10 | 42.238 | 45.432 | 49.239 | 1.00 4 | | 6 | |
| ATOM | 65 | Ο. | LEU A | | 10 | 41.462 | 45.863 | 48.381 | 1.00 4 | | 8 | |
| MOTA | 66 | N . | ASP A | | 11 | 43.052 | 44.408 | 49.025 | 1.00 4 | 13.51 | 7 | |

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Figure 17-2

| ATOM | 67 | CA | ASP | A | 11 | | 43. | 071 | 43.73 | 31 | 47.737 | 1.00 | 47.27 | 6 |
|--------|-------|-----|-------|-----|-----|---|------|-------|-------|----|---------|------|-------|--------|
| ATOM | 68 | CB | ASP | A | 11 | | 44. | 250 | 42.76 | 65 | 47.694 | | 51.03 | 6 |
| MOTA | 69 | CG | ASP | | 11 | | 45. | 579 | 43.47 | 79 | 47.858 | | 54.10 | 6 |
| ATOM | 70 | OD. | 1 ASP | | 11 | | 45. | 944 | 44.28 | 82 | 46.975 | | 55.93 | 8 |
| ATOM | 71 | | 2 ASP | | 11 | | | 255 | 43.25 | | 48.879 | | 57.79 | 8 |
| ATOM | 72 | C | ASP | | 11 | | | 756 | 43.01 | | 47.423 | | 46.36 | 6 |
| ATOM | 73 | Ō | ASP | | 11 | | 41. | 472 | 42.70 | 02 | 46.266 | | 43.49 | 8 |
| ATOM | 74 | N | TYR | | 12 | | | 954 | 42.76 | | 48.456 | | 46.80 | 7 |
| ATOM | 75 | CA | TYR | | 12 | | 39. | 654 | 42:11 | | 48.284 | | 45.92 | 6 |
| ATOM | 76 | CB | TYR | | 12 | | | 953 | 41.94 | | 49.638 | | 41.38 | 6 |
| ATOM | 77 | CG | TYR | | 12 | _ | | 358 | 40.69 | | 50.390 | | 38.82 | 6 |
| ATOM | 78 | | 1 TYR | | 12 | _ | | 531 | 40.72 | | 51.775 | | 37.95 | 6 |
| ATOM | 79 | CE: | | | 12 | | | 869 | 39.56 | | 52.476 | | 36.18 | 6 |
| ATOM | 80 | CD | | | 12 | | | 533 | 39.47 | | 49.721 | | 37.69 | 6 |
| ATOM | 81 | CE | | | 12 | | | 868 | 38.31 | | 50.415 | | 35.83 | 6 |
| ATOM | 82 | CZ | TYR | | 12 | | | 032 | 38.36 | | 51.787- | | 34.10 | 6 |
| ATOM | 83 | OH | TYR | | 12 | | | 339 | 37.21 | _ | 52.470 | | 36.31 | 8 |
| ATOM | 84 | C | TYR | | 12 | | | 786 | 42.96 | | 47.378 | | 46.56 | 6 |
| ATOM | 85 | ō | TYR | | 12 | | | 821 | 42.47 | | 46.791 | | 47.38 | 8 |
| ATOM | 86 | Ŋ | GLY | | 13 | | | 138 | 44.24 | | 47.278 | | 47.28 | 7 |
| ATOM | 87 | CA | GLY | | 13 | | | 385 | 45.16 | | 46.442 | | 46.53 | 6 |
| ATOM | 88 | c | GLY | | 13 | | | 650 | 44.93 | | 44.968 | | 45.60 | 6 |
| ATOM | 89 | ō | GLY | | 13 | | | 895 | 45.40 | | 44.117 | | 43.68 | 8 |
| ATOM | 90 | Ň | LYS | | 4 | | | 725 | 44.21 | | 44.672 | | 46.52 | 7 |
| ATOM | 91 | CA | LYS | | 4 | | | 112 | 43.90 | | 43.296 | | 47.28 | 6 |
| ATOM | 92 | CB | LYS | | 4 | | | 629 | 43.74 | | 43.201 | | 50.22 | 6 |
| ATOM | 93 | CG | LYS | | 4 | | | 396 | 45.04 | | 43.307 | | 57.12 | 6 |
| ATOM | 94 | CD | LYS | | 4 | | 42. | | 46.00 | | 42.161 | | 63.60 | 6 |
| ATOM | 95 | CE | LYS | | 4 | | 42. | 349 | 45.42 | | 40.768 | | 66.65 | 6 |
| ATOM - | 96 | NZ | LYS | | 4 | | 41. | | 44.22 | | 40.387 | | 67.70 | 7 |
| ATOM | 97 | С | LYS | | .4 | | 39. | | 42.64 | 13 | 42.769 | 1.00 | 44.18 | 6 |
| ATOM | 98 | 0 | LYS | | .4 | | 39. | 564 | 42.32 | | 41.585 | | 40.33 | 8 |
| ATOM | 99 | N | TYR | A 1 | 5 | | 38. | 790 | 41.92 | 26 | 43.661 | 1.00 | 43.25 | 7 |
| ATOM | 100 | ÇA | TYR | A 1 | 5 . | | 38. | 145 | 40.66 | 55 | 43.317 | 1.00 | 43.18 | 6 |
| MOTA | 101 | CB | TYR | A 3 | .5 | | 38. | 789 | 39.54 | 17 | 44.142 | 1.00 | 36.88 | 6 |
| ATOM | 102 | ÇG | TYR | A 1 | .5 | | 40. | 302 ' | 39.56 | 50 | 44.053 | 1.00 | 32.96 | 6 |
| ATOM | 103 | CD1 | TYR | A 1 | .5 | | 41. | 084 | 39.10 | 7 | 45.108 | 1.00 | 30.90 | 6 |
| ATOM | 104 | CE1 | TYR | A 1 | .5 | | 42. | 476 | 39.14 | 14 | 45.035 | 1.00 | 30.94 | 6 |
| ATOM | 105 | CD2 | TYR | A 1 | 5 | | 40. | 952 | 40.04 | 19 | 42.912 | 1.00 | 33.01 | 6 |
| MOTA | 106 | CE2 | TYR | A 1 | 5 | | 42. | 341 | 40.09 | 2 | 42.826 | 1.00 | 29.68 | 6 |
| ATOM | 107 | CZ | TYR | a 1 | .5 | | 43. | 098 | 39.63 | | 43.890 | | 30.99 | 6 |
| ATOM | 108 | OH | TYR | A 1 | 5 | | 44. | 471 | 39.67 | | 43.809 | 1.00 | 28.02 | 8 |
| ATOM | 109 | С | TYR | | 5 | | 36. | | 40.77 | | 43.621 | | 45.56 | 6 |
| ATOM | 110 | 0 | TYR | | 5 | | 36. | | 40.15 | | 44.552 | | 45.22 | 8 |
| ATOM | 111 | N | ARG | | 6 | | 35. | | 41.59 | | 42.830 | | 48.81 | 7 |
| MOTA | 112 | CA | ARG | | 6 | | 34. | | 41.81 | | 42.999 | | 53.22 | 6 |
| ATOM | 113 | CB | ARG | | 6 | | 34. | | 43.26 | | 42.654 | | 57.11 | 5 |
| ATOM | 114 | CG | ARG . | | 6 | | 34. | | 44.33 | | 43.490 | | 61.66 | 6 |
| ATOM | 115 | CD | ARG . | | 6 | | 34. | | 44.40 | | 44.886 | | 67.04 | 6 |
| ATOM | 116 | NE | ARG . | | 6 | | 34. | | 45.59 | | 45.569 | | 73.59 | 7 |
| MOTA | 117 | | ARG . | | 6 | - | 34. | | 46.83 | | 45.141 | | 75.03 | 6 |
| | . 118 | | | | | | 33.5 | | 47.06 | | 44.033 | | 73.03 | 7 |
| ATOM | 119 | | ARG . | | | | 35. | | 47.85 | | 45.808 | | 75.79 | 7 |
| MOTA | 120 | C | ARG . | | | | 33. | | | | 42.080 | | 51.79 | 6 |
| ATOM | 121 | 0 | ARG . | | | | 34. | | 40.59 | | 40.970 | | 50.89 | . 3 |
| ATOM | 122 | N | TYR | | | | 32.5 | | 40.46 | | 42.552 | | 50.19 | |
| MOTA | 123 | CA | TYR : | | | | 31. | | 39.63 | | 41.733 | | 49.60 | 6 |
| ATOM | 124 | CB | TYR A | | | | 30.5 | | 39.11 | | 42.528 | | 45.80 | 6 |
| ATOM | 125 | CG | TYR A | | | | 30.8 | | 37.89 | | 43.365 | | 42.01 | 6 |
| ATOM | 126 | | TYR . | | | | 31. | | 37.93 | | 44.438 | | 42.45 | 6 |
| ATOM | 127 | | TYR 2 | | | | 31.9 | | 36.78 | | 45.193 | | 43.36 | 6 |
| ATOM | 128 | CD2 | TYR 3 | | | | 30.3 | | 36.68 | _ | 43.062 | | 39.89 | 6 |
| ATOM | 129 | CE2 | TYR : | | | | 30. | | 35.52 | | 43.803 | | 40.56 | 6 |
| ATOM | 130 | CZ | TYR : | | | | 31.3 | | 35.57 | | 44.869 | | 41.98 | 6 |
| ATOM | 131 | OH | TYR : | | | | 31.6 | | 34.43 | | 45.598 | | 34.66 | 8 6 |
| ATOM | 132 | C | TYR A | 1 | 1 | | 31.2 | 445 | 40.54 | ′ | 40.622 | 1.00 | 51.88 | O |

| ATOM | 133 | 0 | TYR A | 17 | | 31.332 | 41.772 | 40.726 | 1.00 47.86 | 8 |
|--------|-----|-----|---------|------|---|--------|---------------------|----------------|--------------|-----|
| | 134 | N | PRO A | | | 30.730 | 39.964 | 39.534 | 1.00 54.38 | 7 |
| ATOM | | | | | | | | | | |
| ATOM | 135 | CD | PRO A | 18 | | 30.548 | 38.545 | 39.190 | 1.00 54.21 | 6 |
| MOTA | 136 | CA. | PRO A | 18 | | 30.243 | 40.809 | 38.449 | 1.00 56.43 | 6 |
| ATOM | 137 | CB | PRO A | 18 | | 29.601 | 39.792 | 37.496 | 1.00 56.84 | 6 |
| ATOM - | 138 | CG | PRO A | 18 | | 29.260 | 38.613 | 38.426 | 1.00 56.46 | 6 |
| | | | | | | | | | | |
| MOTA | 139 | С | PRO A | 18 | | 29.273 | 41.891 | 38.932 | 1.00 58.74 | 6 |
| MOTA | 140 | О | PRO A | . 18 | | 28.791 | 41.861 | 40.066 | 1.00 55.72 | 8 |
| ATOM | 141 | N | LYS A | 19 | | 29.017 | 42.851 | 38.052 | 1.00 62.10 | 7 |
| ATOM | 142 | CA | LYS A | 19 | | 28.127 | 43.973 | 38.314 | 1.00 64.85 | 6 |
| | | | | | | 27.972 | 44.781 | | | |
| ATOM | 143 | CB | LYS A | 19 | | | | 37.022 | 1.00 69.74 | 6 |
| MOTA | 144 | CG | LYS A | | | 28.008 | 43.925 | 35.740 | 1.00 74.99 | 5 |
| ATOM | 145 | CD | LYS A | 19 | - | 26.895 | 42.881 | 35.668 | - 1.00 78.18 | 6 |
| MOTA | 146 | CE | LYS A | 19 | | 26.981 | 42.010 | 34.420 | 1.00 80.24 | · б |
| MOTA | 147 | NZ | LYS A | 19 | | 25.867 | 41.010 | 34.361 | 1.00 81.13 | 7 |
| | | | | | | 26.750 | 43.619 | | 1.00 64.77 | |
| ATOM | 148 | C | LYS. A | 19 | | | | 38.869 | | 6 |
| ATOM | 149 | 0 | LYS A | 19 | | 26.414 | 43.961 | 40.001 | 1.00 66.50 | .8 |
| ATOM | 150 | N | ASN A | 20 | | 25.957 | 42.933 | 38.062 | 1.00 63.75 | 7 |
| ATOM | 151 | CA | ASN A | 20 | | 24.612 | 42.556 | 38.439 | 1.00 62.96 | 6 |
| ATOM | 152 | CB | ASN A | 20 | | 23.870 | 42.031 | 37.208 | 1.00 67.42 | 6 |
| | 153 | CG | ASN A | 20 | | 22.392 | 41.833 | 37.459 | | |
| MOTA | | | | | | | | | 1.00 72.29 | |
| ATOM | 154 | OD1 | | 20 | | 21.666 | 42.785 | 37.772 | 1.00 75.25 | . 8 |
| ATOM | 155 | ND2 | ASN A | 20 | | 21.931 | 40.594 | 37.322 | 1.00 74.38 | 7 |
| ATOM | 156 | С | ASN A | 20 | | 24.602 | 41.512 [.] | 39.5 47 | 1.00 61.30 | 6 |
| ATOM | 157 | 0 | ASN A | 20 | | 23.629 | 40.773 | 39.698 | 1.00 61.49 | 8 |
| ATOM | 158 | N | HIS A | 21 | | 25.681 | 41.444 | 40.321 | 1.00 57.30 | 7 |
| | | | | | | 25.755 | | | | |
| ATOM | 159 | CA | HIS A | 21 | | | 40.480 | 41.418 | 1.00 54.68 | 6 |
| ATOM | 160 | CB | HIS A | 21 | | 27.071 | 39.700 | 41.373 | 1.00 52.63 | 6 |
| ATOM | 161 | CG | HIS A | 21 | | 27.058 | 38.449 | 42.195 | 1.00 49.39 | 6 |
| ATOM | 162 | CD2 | HIS A | 21 | | 27.336 | 38.236 | 43.503 | 1.00 49.39 | 6 |
| ATOM | 163 | ND1 | HIS A | 21 | | 26.664 | 37.229 | 41.686 | 1.00 48.27 | 7 |
| ATOM | 164 | | HIS A | 21 | | 26.704 | 36.320 | 42.643 | 1.00 48.16 | 6 |
| | 165 | | HIS A | 21 | | 27.108 | 36.905 | 43.757 | 1.00 47.33 | 7 |
| ATOM | | | | | | | - | | | |
| ATOM | 166 | C | HIS A | 21 | | 25.664 | 41.215 | 42.760 | 1.00 52.89 | 6 |
| MOTA | 167 | 0 | HIS A | 21 | | 26.295 | 42.256 | 42.947 | 1.00 52.52 | 8 |
| ATOM | 168 | N | PRO A | 22 | | 24.880 | 40.679 | 43.713 | 1.00 50.81 | 7 |
| ATOM | 169 | CD | PRO A | 22 | | 24.076 | 39.444 | 43.661 | 1.00 48.50 | 6 |
| ATOM | 170 | CA | PRO A | 22 | | 24.734 | 41.310 | 45.029 | 1.00 48.02 | 6 |
| ATOM | 171 | CB | PRO A | 22 | | 23.860 | 40.308 | 45.783 | 1.00 47.45 | 6 |
| | 172 | CG | PRO A | -22 | | 22.990 | 39.754 | 44.667 | 1.00 47.76 | 6 |
| MOTA | | | | | | | 41.558 | | | 6 |
| ATOM | 173 | С | PRO A | 22 | | 26.074 | | 45.727 | 1.00 46.48 | |
| MOTA | 174 | o | PRO A | 22 | | 26.164 | 42.405 | 46.615 | 1.00 45.69 | 8 |
| ATOM | 175 | N | LEU A | 23 | | 27.107 | 40.816 | 45.318 | 1.00 44.97 | 7 |
| ATOM | 176 | CA | LEU A | 23 | | 28.441 | 40.949 | 45.906 | 1.00 41.31 | 6 |
| ATOM | 177 | CB | LEU A | 23 | | 29.076 | 39.569 | 46.131 | 1.00 39.22 | 6 |
| ATOM | 178 | CG | LEU A | 23 | | 28.264 | 38.561 | 46.953 | 1.00 37.71 | 6 |
| | | | | | | | | | | |
| ATOM | 179 | | LEŲ A | 23 | | 29.075 | 37.288 | 47.157 | 1.00 35.07 | 6 |
| ATOM | 180 | CD2 | LEU A | 23 | | 27.896 | 39.165 | 48.292 | 1.00 36.90 | 6 |
| ATOM | 181 | С . | LEU A | 23 | | 29.334 | 41.789 | 45.003 | 1.00 40.14 | 6 |
| ATOM | 182 | 0 | LEU A | 23 | | 30.556 | 41.614 | 44.951 | 1.00 39.00 | 8 |
| ATOM | 183 | N | LYS A | 24 | | 28.706 | 42.705 | 44.284 | 1.00 39.67 | 7 |
| | | | | | | 29.430 | 43.590 | | .1.00 42.88 | _ |
| ATOM | 184 | CA | LYS A | 24 | | | | | | 6 |
| ATOM | 185 | CB | LYS A | 24 | | 28.480 | 44.120 | 42.323 | 1.00 40.24 | 6 |
| ATOM | 186 | CG | LYS A | 24 | | 28.949 | 45.362 | 41.610 | 1.00 44.08 | 6 |
| ATOM | 187 | CD | LYS A | 24 | | 28.247 | 46.600 | 42.166 | 1.00 44.47 | 6 |
| ATOM | 188 | CE | LYS A | 24 | | 26.732 | 46.492 | 41.968 | 1.00 43.23 | 6 |
| | | | | | | | | | 1.00 39.79 | 7 |
| ATOM | 189 | NZ | LYS A | 24 | | 25.989 | 47.717 | 42.362 | | |
| ATOM | 190 | С | LYS A | 24 | | 30.031 | 44.723 | 44.217 | 1.00 43.70 | 6 |
| ATOM | 191 | 0 | LYS A | 24 | | 31.027 | 45.332 | 43.817 | 1.00 47.22 | 8 |
| ATOM | 192 | N | ILE A | 25 | | 29.431 | 44.976 | 45.378 | 1.00 42.27 | 7 |
| ATCM | 193 | CA | ILE A | 25 | | 29.870 | 46.035 | 46.289 | 1.00 39.86 | 6 |
| | 194 | CB | ILE A | 25 | | 28.763 | 46.407 | 47.306 | 1.00 37.72 | 6 |
| ATOM | | CG2 | | 25 | | 27.539 | 46.953 | 46.580 | 1.00 39.67 | 6 |
| ATOM | 195 | | ILE A | | | | | | 1.00 35.25 | 6 |
| ATCM | 196 | | ILE A | 25 | | 28.410 | 45.168 | 48.145 | | |
| ATOM | 197 | CDI | ILE . A | 25 | | 27.301 | 45.368 | 49.151 | 1.00 31.74 | 6 |
| ATCM | 198 | С | ILE A | 25 | | 31.078 | 45.625 | 47.112 | 1.00 40.23 | 6 |

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| MOTA | 199 | 0 | ILE | A 25 | | 31.419 | 44.441 | 47.198 | 1.00 38.90 | 8 |
|--------|-----|-------------|-------|-------------|---|---------|--------|--------|------------|-----|
| ATOM | 200 | N | PRO | | | 31.762 | 46.616 | 47.709 | 1.00 40.18 | 7 |
| | 201 | CD | PRO | | | | 48.051 | 47.533 | | |
| ATOM | | | | _ | | 31.523 | | | 1.00 40.58 | 6 |
| ATOM | 202 | CA | PRO | | | 32.939 | 46.437 | 48.558 | 1.00 38.31 | 6 |
| MOTA | 203 | CB | PRO | A 26 | | 33.478 | 47.860 | 48.688 | 1.00 37.14 | 6 |
| MOTA | 204 | CG | PRO | A 26 | | 32.940 | 48.537 | 47.458 | 1.00 38.77 | 6 |
| ATOM | 205 | С | PRO | A 26 | | 32.433 | 45.903 | 49.891 | 1.00 37.32 | 6 |
| MOTA | 206 | 0 | PRO | | | 31.416 | 46.372 | 50.412 | 1.00 32.70 | 8 |
| ATOM | 207 | N | ARG | | | 33.134 | 44.930 | 50.452 | 1.00 36.54 | 7 |
| | | | | | | _ | | 51.711 | | |
| MOTA | 208 | CA | ARG | | | 32.685 | 44.359 | | 1.00 37.39 | 6 |
| MOTA | 209 | CB | ARG | | | 32.116 | 42.952 | 51.455 | 1.00 35.29 | 6 |
| MOTA | 210 | CG | ARG | | | 31.047 | 42.956 | 50.355 | 1.00 32.69 | 6 |
| ATOM | 211 | $^{\rm CD}$ | ARG | A 27 | | 30.507 | 41.573 | 49.956 | 1.00 33.87 | 6 |
| ATOM | 212 | NE | ARG | A 27 | | 29.757 | 40.909 | 51.021 | 1.00 36.16 | 7 |
| ATOM | 213 | CZ | ARG | | | 30.293 | 40.132 | 51.959 | 1.00 37.11 | 6 |
| ATOM | 214 | | ARG | | | 31.604 | 39.903 | 51.976 | 1.00 34.42 | 7 |
| ATOM | 215 | | ARG | | | 29.516 | 39.597 | 52.896 | 1.00 33.67 | 7 |
| | | | | | | | | 52.732 | | |
| ATOM | 216 | C | ARG | | | 33.813 | 44.329 | | 1.00 36.35 | 6 |
| MOTA | 217 | 0 | ARG | | | 33.881 | 45.188 | 53.610 | 1.00 35.77 | 8 |
| ATOM | 218 | N | VAL | A 28 | | 34.703 | 43.351 | 52.607 | 1.00 34.93 | 7 |
| MOTA | 219 | CA | VAL | A 28 | | 35.810 | 43.230 | 53.537 | 1.00 34.00 | 6 |
| ATOM | 220 | CB | VAL | A 28 | | 36.633 | 41.954 | 53.252 | 1.00 36.21 | 6 |
| MOTA | 221 | CG1 | VAL | | | 37.574 | 41.652 | 54.424 | 1.00 33.59 | 6 |
| ATOM | 222 | | VAL | | | 35.696 | 40.790 | 52.992 | 1.00 37.05 | 6 |
| | 223 | C | VAL | | | 36.712 | 44.454 | 53.423 | 1.00 37.03 | 6 |
| MOTA | 224 | | VAL | | | | 44.959 | 54.427 | | |
| ATOM | | 0 | | | | 37.216 | | | 1.00 31.45 | 8 |
| MOTA | 225 | N | SER | | | 36.908 | 44.936 | 52.199 | 1.00 33.12 | |
| ATOM | 226 | CA | SER | _ | | 37.751 | 46.111 | 51.967 | 1.00 32.03 | 6 |
| MOTA | 227 | CB | SER | | | 38.205 | 46.181 | 50.499 | 1.00 31.77 | 6 |
| MOTA | 228 | OG | SER | A 29 | | 37, 113 | 46.223 | 49.600 | 1.00 30.80 | 8 |
| ATOM | 229 | С | SER | A 29 | | 37.003 | 47.380 | 52.353 | 1.00 30.16 | 6 |
| ATOM | 230 | 0 | SER | A 29 | | 37.604 | 48.404 | 52.650 | 1.00 28.70 | 8 |
| ATOM | 231 | N | LEU | | | 35.682 | 47.310 | 52.352 | 1.00 32.43 | 7 |
| MOTA | 232 | CA | LEU | | | 34.900 | 48:465 | 52.745 | 1.00 34.56 | 6 |
| ATOM . | 233 | CB | LEU | | | 33.463 | 48.358 | 52.221 | 1.00 36.44 | 6 |
| | 234 | CG | LEU | | | 32.508 | 49.513 | 52.560 | 1.00 36.79 | 6 |
| MOTA | | | | | | | | | | |
| ATOM | 235 | | LEU . | | | 32.070 | 49.446 | 54.012 | 1.00 36.73 | 6 |
| MOTA | 236 | | LEU . | | | 33.202 | 50.840 | 52.256 | 1.00 37.84 | 6 |
| MOTA | 237 | С | LEU . | | | 34.902 | 48.527 | 54.262 | 1.00 34.89 | 6 |
| MOTA | 238 | 0 | LEU . | <i>y</i> 30 | | 35.033 | 49.601 | 54.841 | 1.00 37.58 | 8 |
| ATOM | 239 | N | LEU . | A 31 | • | 34.761 | 47.366 | 54.897 | 1.00 34.07 | 7 |
| ATOM | 240 | CA | LEU . | A 31 | | 34.743 | 47.276 | 56.350 | 1.00 34.85 | 6 |
| ATOM | 241 | CB | LEU . | A 31 | | 34.768 | 45.808 | 56.791 | 1.00 36.37 | 6 |
| ATOM | 242 | CG | LEU . | | | 34.459 | 45.471 | 58.261 | 1.00 36.04 | 6 |
| ATOM | 243 | | LEU | | | 34.841 | 44.027 | 58.532 | 1.00 35.13 | 6 |
| ATOM | 244 | | LEU | | | 35.228 | 46.357 | 59.194 | 1.00 35.86 | . 6 |
| | 245 | C | LEU | | | 35.976 | 47.994 | 56.894 | 1.00 36.43 | . ē |
| MOTA | | | | | | 35.855 | 49.035 | 57.544 | | 8 |
| ATOM | 246 | 0 | LEU | | | | | | 1.00 35.87 | |
| ATOM | 247 | N | LEU Z | | | 37.157 | 47.426 | 56.635 | 1.00 37.76 | 7 |
| ATCM | 248 | CA | LEU A | | | 38.420 | 48.015 | 57.087 | 1.00 36.82 | 5 |
| ATOM | 249 | CB | LEU A | | | 39.611 | 47.318 | 56.418 | 1.00 36.37 | 6 |
| ATOM | 250 | CG | LEU 3 | A 32 | | 40.030 | 45.888 | 56.774 | 1.00 39.11 | 6 |
| ATOM! | 251 | CD1 | LEU A | A 32 | | 41.117 | 45.420 | 55.815 | 1.00 35.16 | 6 |
| ATOM | 252 | | LEU 2 | | | 40.538 | 45.830 | 58.214 | 1.00 37.73 | 6 |
| ATOM | 253 | C | LEU A | | | 38.500 | 49.513 | 56.780 | 1.00 34.84 | 6 |
| | 254 | õ | LEU A | | | 38.846 | 50.326 | 57.644 | 1.00 36.58 | 8 |
| ATOM | | | | | | | | | | 7 |
| ATOM | 255 | N | ARG A | | | 38.184 | 49.877 | 55.545 | 1.00 31.37 | |
| ATOM | 256 | CA | ARG A | | | 38.247 | 51.270 | 55.150 | 1.00 32.53 | 6 |
| ATOM | 257 | CB | ARG A | | | 37.927 | 51.398 | 53.662 | 1.00 31.52 | 6 |
| ATCM | 258 | CG | ARG 2 | 33 | | 38.481 | 52.652 | 53.042 | 1.00 35.88 | 6 |
| ATOM | 259 | CD | ARG A | 33 | | 38.107 | 52.752 | 51.581 | 1.00 43.44 | 6 |
| ATCM | 260 | NE | ARG 2 | | | | 51.583 | 50.811 | 1.00 48.37 | 7 |
| ATCM | 261 | CZ | ARG A | | | 38.348 | 51.469 | 49.497 | 1.00 52.27 | 6 |
| ATOM | 262 | | ARG ? | | | 37.771 | 52.459 | 48.823 | 1.00 51.75 | 7 |
| | 263 | NH2 | ARG A | | | 38.739 | 50.369 | 48.858 | 1.00 51.08 | 7 |
| ATCM | | | | | | 200723 | | | | 6 |
| ATCM | 264 | C | ARG A | 33 | | 37.274 | 52.102 | 55.989 | 1.00 32.32 | |

| MOTA | 265 | 0 | ·ARG A | . 33 | | 37.471 | 53.299 | 56.196 | 1.00 29.23 | 8 |
|--------|-------|-----|---------|------|---|--------|--------|--------|-------------|-----|
| ATOM | 266 | N | PHE A | 34 | | 36.231 | 51.445 | 56.484 | 1.00 32.58 | 7 |
| | 267 | | | | | 35.216 | 52.096 | 57.304 | 1.00 32.69 | |
| MOTA | | | | | | | | | | 6 |
| MOTA | 268 | | PHE A | | | 33.952 | 51.232 | 57.359 | 1.00 31.22 | 6 |
| MOTA | 269 | CG | PHE A | 34 | | 32.838 | 51.825 | 58.183 | 1.00 28.74 | 6 |
| ATOM | 270 | CD | 1 PHE A | 34 | | 32.085 | 52.888 | 57.700 | 1.00 22.76 | 6 |
| | 271 | CD | | | | 32.551 | 51.322 | 59.456 | 1.00 28.09 | 6 |
| MOTA | | | | | | | | | | |
| MOTA | 272 | | 1 PHE A | | | 31.061 | 53.441 | 58.472 | 1.00 23.70 | 6 |
| MOTA | 273 | CE: | 2 PHE A | 34 | | 31.524 | 51.873 | 60.235 | 1.00 24.59 | 6 |
| ATOM | 274 | CZ | PHE A | 34 | | 30.781 | 52.929 | 59.741 | 1.00 21.39 | 6 - |
| ATOM | 275 | C | PHE A | | | 35.734 | 52.319 | 58.719 | 1.00 33.45 | 6 |
| | 276 | | | | | 35.635 | 53.425 | 59.258 | | |
| ATOM | | 0 | PHE A | | | | | | 1.00 35.49 | 8 |
| ATOM | 277 | N | LYS A | | | 36.276 | 51.264 | 59.323 | 1.00 34.52 | 7 |
| MOTA | 278 | CA | LYS A | 35 | | 36.805 | 51.360 | 60.678 | 1.00 36.51 | 6 |
| ATOM | 279 | CB | LYS A | . 35 | | 37.118 | 49.977 | 61.235 | 1.00 36.47 | 6 |
| MOTA | 280 | CG | LYS A | _ | | 35.912 | 49.074 | 61.343 | 1.00 40.81 | 6 |
| | | | | | | | _ | | | |
| ATOM | 281 | CD | LYS A | - | | 36.246 | 47.801 | 62.090 | 1.00 44.10 | 6 |
| MOTA | 282 | CE | LYS A | 35 | | 37.347 | 47.029 | 61.402 | 1.00 47.46 | 6 |
| ATOM | 283 | NZ | LYS A | 35 | | 38.601 | 47.823 | 61.276 | 1.00 53.53 | 7 |
| ATOM | 284 | С | LYS A | 35 | | 38.054 | 52.222 | 60.735 | 1.00 36.61 | 6 |
| ATOM | 285 | Õ | LYS A | 35 | | 38.352 | 52.824 | 61.766 | 1.00 .36.78 | 8 |
| | | | | | | | | | | |
| ATOM | 286 | N | ASP A | 3,6 | | 38.794 | 52.267 | 59.635 | 1.00 36.27 | 7 |
| MOTA | 287 | CA | ASP A | 36 | | 39.980 | 53.090 | 59.592 | 1.00 39.71 | 6 |
| MOTA | 288 | CB | ASP A | 36 | | 40.679 | 52.937 | 58.239 | 1.00 44.78 | 6 |
| MOTA | 289 | CG | ASP A | 36 | | 41.863 | 53.892 | 58.075 | 1.00 47.10 | 6 |
| ATOM | 290 | | ASP A | 36 | | 42.803 | 53.852 | 58.906 | 1.00 44.02 | 8 |
| | 291 | | ASP A | 36 | | 41.843 | 54.682 | 57.106 | 1.00 48.43 | 8 |
| MOTA | | | | | | | | | | |
| MOTA | 292 | С | ASP A | 36 | • | | 54.530 | 59.789 | 1.00 39.99 | 6 |
| MOTA | 293 | 0 | ASP A | 36 | | 40.023 | 55.258 | 60.636 | 1.00 40.76 | 8 |
| ATOM | 294 | N | ALA A | 37 | | 38.506 | 54.919 | 59.007 | 1.00 38.59 | 7 |
| ATOM | 295 | CA | ALA A | 37 | | 37.939 | 56.258 | 59.066 | 1.00 37.14 | 6 |
| | 296 | CB | ALA A | 37 | | 36.857 | 56.402 | 58.000 | 1.00 35.85 | 6 |
| MOTA | | | | | | | | | | |
| MOTA | 297 | C | ALA A | 37 | | 37.354 | 56.549 | 60.446 | 1.00 38.34 | 6 |
| MOTA | 298 | 0 | ALA A | 37 | | 37.391 | 57.687 | 60.928 | 1.00 37.32 | 8 |
| MOTA | 299 | N | MET A | 38 | | 36.809 | 55.518 | 61.079 | 1.00 36.19 | 7 |
| ATOM | 300 | CA | MET A | 38 | | 36.213 | 55.674 | 62.397 | 1.00 36.80 | 6 |
| ATOM | 301 | CB | MET A | 38 | | 35,141 | 54.598 | 62.606 | 1.00 37.38 | 6 |
| | | .ce | | 38 | - | | 54.717 | 61.673 | 1.00 37.60 | 6 |
| MOTA | 302 | | MET A | | | 33.938 | - | | | |
| MOTA | 303 | SD | MET A | 38 | | 32.887 | 56.165 | 61.999 | 1.00 33.61 | 16 |
| ATOM . | 304 | CE | MET A | 38 | | 32.398 | 55.824 | 63.680 | 1.00 35.60 | 6 |
| ATOM | 305 | С | MET A | 38 | | 37.262 | 55.582 | 63.502 | 1.00 35.84 | 6 |
| MOTA | 306 | 0 | MET A | 38 | | 36.937 | 55.688 | 64.692 | 1.00 34.89 | 8 |
| ATOM | 307 | N | ASN A | 39 | | 38.518 | 55.400 | 63.100 | 1.00 33.83 | 7 |
| | | | | 39 | | | 55.264 | 64.044 | | 6 |
| ATOM | 308 | CA | ASN A | | | 39.626 | | | - · · · | |
| ATOM | 309 | CB | ASN A | 39 | | 39.897 | 56.582 | 64.775 | 1.00 32.48 | 6 |
| ATOM | 310 | CG | ASN A | 39 | | 40.213 | 57.717 | 63.825 | 1.00 32.34 | 6 |
| MOTA | 311 | OD1 | ASN A | 39 | | 41.128 | 57.621 | 63.009 | 1.00 31.85 | 8 |
| ATOM | 312 | ND2 | | 39 | | 39.455 | 58.800 | 63.924 | 1.00 30.92 | 7 |
| | 313 | c | ASN A | 39 | | 39.253 | 54.183 | 65.045 | 1.00 36.87 | 6 |
| MOTA | | | | | | | | | | |
| MOTA | 314 | 0 | ASN A | 39 | | 39.403 | 54.357 | 66.260 | 1.00 36.60 | 8 |
| ATOM | 315 | N | LEU A | 40 | | 38.752 | 53.067 | 64.518 | 1.00 37.48 | 7 |
| MOTA | 316 | CA | LEU A | 40 | | 38.341 | 51.933 | 65.336 | 1.00 39.66 | 6 |
| ATOM | 317 | CB | LEU A | 40 | | 36.863 | 51.622 | 65.086 | 1.00 41.35 | 6 |
| | . 318 | ĊĠ | LEU A | 40 | | 35.858 | 52.712 | 65.476 | 1.00 42.69 | 6 |
| | | | | | | | | | | |
| ATOM | 319 | | LEU A | 40 | | 34.448 | 52.261 | 65.111 | 1.00 45.05 | 6 |
| MOTA | 320 | CD2 | LEU A | 40 | | 35.951 | 52.989 | 66.966 | 1.00 39.44 | 6 |
| ATOM | 321 | С | LEU A | 40 | | 39.184 | 50.687 | 65.058 | 1.00 39.79 | 6 |
| ATOM | 322 | 0 | LEU A | 40 | | 38.804 | 49.575 | 65.434 | 1.00 36.88 | 8 |
| | | | ILE A | | | 40.337 | 50.889 | 64.420 | 1.00 40.50 | 7 |
| MOTA | 323 | N | | 41 | | | | | | |
| MOTA | 324 | CA | ILE A | 41 | • | 41.237 | 49.790 | 64.068 | 1.00 41.39 | 6 |
| ATOM | 325 | CB | ILE A | 41 | | 40.780 | 49.141 | 62.724 | 1.00 39.24 | 6 |
| ATOM | 326 | CG2 | ILE A | 41 | | 41.017 | 50.103 | 61.564 | 1.00 36.97 | 6 |
| ATOM | 327 | CG1 | | 41 | | 41.513 | 47.824 | 62.482 | 1.00 36.76 | 6 |
| | | | ILE A | 41 | | 41.085 | 46.715 | 63.403 | 1.00 35.59 | 6 |
| ATOM | 328 | | | | | | | | | 6 |
| MOTA | 329 | C | ILE A | 41 | | 42.684 | 50.295 | 63.913 | 1.00 44.37 | |
| ATOM | 330 | 0 | ILE A | 41 | | 42.927 | 51,328 | 63.277 | 1.00 46.01 | 8 |
| | | _ | | • | • | | | | | |

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| MOTA | 331 | N | ASP | A 42 | 43. | 646 | 49.582 | 64.497 | 1.00 | 45.19 | 7 |
|--------------|-------------|---------|---------|----------|--------------|------|------------------|------------------|------|----------------|--------|
| ATOM | 332 | CA | ASP . | A 42 | | 049 | 49.982 | 64.372 | | 45.62 | 6 |
| MOTA | 333 | CB | ASP . | A 42 | 45. | 716 | 50.090 | 65.742 | | 45.17 | ě |
| MOTA | 334 | CG | ASP . | A 42 | 44. | 966 | 51.005 | 66.682 | | 44.43 | 6 |
| ATOM | 335 | OD: | l ASP . | A 42 | 44. | 731 | 52.177 | 66.322 | | 39.84 | 8 |
| ATOM | 336 | OD: | 2 ASP | A 42 | 44. | 612 | 50.546 | 67.787 | | 48.50 | 8 |
| MOTA | 337 | C | ASP . | A 42 | 45. | 750 | 48.915 | 63.551 | | 48.47 | 6 |
| MOTA | 338 | 0 | ASP . | A 42 | 45. | 316 | 47.757 | 63.547 | 1.00 | 49.85 | 8 |
| MOTA | 339 | N | GLU / | | 46. | 830 | 49.288 | 62.864 | 1.00 | 49.24 | 7 |
| MOTA | 340 | CA | GLU 1 | | 47. | 553 | 48.325 | 62.028 | 1.00 | 50.79 | 6 |
| ATOM | 341 | CB | GLU A | | | 820 | 48.956 | 61.431 | | 49.90 | 6 |
| ATOM | 342 | CG | GLU A | | | 544 | 50.029 | 60.378 | 1.00 | 57.20 | 6 |
| ATOM | 343 | CD | GLU A | | | 808 | 50.537 | 59.690 | 1.00 | 59.56 | 6 |
| ATOM | 344 | OE | | | | 517 | 49.721 | 59.061 | | 65.05 | 8 |
| MOTA | 345 | OE2 | | | | 095 | 51.750 | 59.772 | 1.00 | 57.82 | 8 |
| ATOM | 346 | C | GLU / | | | 918 | 47.020 | 62.733 | 1.00 | 49.73 | 6 |
| ATOM | 347 348 | N O | GLU A | | • | 813 | 45.943 | 62.149 | | 49.18 | 8 |
| ATOM ATOM | 349 | CA | LYS A | | | 324 | 47.118 | 63.992 | | 49.40 | 7 |
| ATOM | 350 | CB | LYS A | | 49. | | 45.949 | 64.762 | | 49.09 | 6 |
| MOTA | 351 | CG | LYS A | | 50. | | 46.418 47.421 | 66.093 65.899 | | 52.46 | 6 |
| ATOM | 352 | CD | LYS A | | 51. | | 47.749 | 67.201 | | 55.75 58.74 | 6 |
| ATOM | 353 | CE | LYS A | | 52. | | 48.704 | 66.949 | | 58.48 | 6 6 |
| ATOM | 354 | NZ | LYS A | | 53. | | 48.968 | 68.176 | | 58.95 | 7 |
| ATOM | 355 | С | LYS A | | 47. | | 44.897 | 64.994 | | 47.63 | 6 |
| ATOM | 356 | 0 | LYS A | | 47. | | 43.738 | 65.290 | | 45.13 | 8 |
| ATOM | 357 | N | GLU A | 45 | 46. | | 45.298 | 64.854 | | 45.25 | 7 |
| ATOM | 358 | CA | GLU A | 45 | .45. | 268 | 44.374 | 65.046 | | 43.09 | 6 |
| MOTA | 359 | CB | GLU A | | 44. | 024 | 45.143 | 65.514 | | 41.19 | 6 |
| ATOM- | 360 | ÇG | GLU A | | 44. | | 45.859 | 66.844 | 1.00 | 36.83 | 6 |
| ATOM | 361 | CD | GLU A | | 43. | | 46.741 | 67.204 | | 38.92 | 6 |
| ATOM | 362 | | GLU A | | 42. | | 47.701 | 66.447 | | 37.30 | 8 |
| ATOM | 363 | | GLU A | | 42. | | 46.479 | 68.253 | | 36.33 | 8 |
| ATOM | 364 | Ċ | GLU A | | 44. | | 43.660 | 63.726 | | 43.04 | 6 |
| ATOM . | 365. 366 | 0 | .GLU A | | 44. | | | 63.699 | | 45.03 | 8 |
| ATOM ATOM | 367 | N CA | LEU A | | 45. 45. | | 44.341 | 62.632 | | 40.29 | 7 |
| ATOM | 368 | CB | LEU A | | 44. | | 43.823 44.990 | 61.299 60.331 | | 37.16 | 6 |
| ATOM | 369 | CG | LEU A | | 44. | | 44.658 | 58.845 | | 37.86 39.22 | 6 6 |
| MOTA | 370 | | LEU A | | 43.1 | | 43.726 | 58.563 | | 40.68 | 6 |
| ATOM | 371 | | LEU A | | 44. | ž . | 45.964 | 58.080 | | 41.62 | 6 |
| ATOM | 372 | С | LEU A | | 46. | | 42.860 | 60.774 | | 36.54 | 6 |
| ATOM | 373 | 0 | LEU A | 46 | 47.2 | | 43.192 | 60.698 | | 39.86 | 8 |
| ATOM | 374 | N | ILE A | 47 | 45.0 | 646 | 41.662 | 60.406 | 1.00 | 33.49 | 7 |
| ATOM | 375 | CA | ILE A | 47 | 46.5 | | 40.657 | 59.844 | 1.00 | 30.51 | 6 |
| ATOM | 376 | CB | ILE A | 47 | 46.3 | | 39.253 | 60.491 | 1.00 | 34.31 | 6 |
| ATOM | 377 | CG2 | ILE A | 47 | 47.3 | | 38.262 | 59.930 | | 32.16 | 6 |
| MOTA | 378 | | ILE A | 47 | 46.5 | | 39.328 | 62.010 | | 32.65 | 6 |
| MOTA | 379 | | ILE A | | 47.8 | | 39.846 | 62.448 | | 38.97 | 6 |
| MOTA | 380 | C | ILE A | 47 | 46.1 | | 10.570 | 58.362 | | 28.36 | 6 |
| ATOM | 381 382 | 0 | ILE A | 47 | 45.0 | | 10.342 | 58.003 | | 26.11 | 8 |
| ATOM ATOM | 383 | N CA | LYS A | 48 48 | 47.1 46.9 | | 10.772 | 57.504 | | 27.77 | 7 |
| ATOM | 384 | CB | LYS A | 48 | 48.2 | | 0.713 | 56.056 | | 25.80 23.91 | 6 |
| MOTA | 385 | CG | LYS A | 48 | 48.0 | | 11.087 11.273 | 55.308 53.811 | | 24.90 | 6 6 |
| ATOM | 386 | CD | LYS A | 48 | 49.3 | | 11.352 | 53.091 | | 26.39 | 6 |
| ATOM | 387 | CE | LYS A | 48 | 49.2 | | 1.864 | 51.679 | | 27.71 | 6 |
| ATOM | 388 | NZ | LYS A | 48 | 48.7 | | 13.275 | 51.696 | | 32.59 | 7 |
| ATOM | 389 | c | LYS A | 48 | 46.5 | | 9.299 | 55.654 | | 26.32 | 6 |
| ATCM | 390 | ō | LYS A | 48 | 47.0 | | 8.325 | 56.235 | | 27.85 | 8 |
| ATOM | 391 | N | SER A | 49 | 45.7 | | 9.183 | 54.653 | | 24.73 | 7 |
| MOTA | 392 | CA | SER A | 49 | 45.2 | | 7.876 | 54.205 | | 27.36 | 6 |
| ATOM | 393 | CB | SER A | 49 | 43.9 | | 7.979 | 53.479 | | 25.04 | 6 |
| ATOM | 394 | OG | SER A | 49 | 42.9 | | 8.329 | 54.373 | 1.00 | 26.94 | 8 |
| ATOM | 395 | С | SER A | 49 | 46.3 | 22 3 | 7.211 | 53.293 | 1.00 | 28.97 | 6 |
| ATOM | 396 | 0 | SER A | 49 | 47.0 | | 7.885 | 52.612 | | 31.89 | 8 |

| ATOM | 397 | 7 N | ARG | Α | 50 | | 46.319 | 35.879 | 53.296 | 1.00 29.71 | 7 |
|--------------|------------|-----------|--------|----------|----|---|------------------|------------------|------------------|--------------------------|--------|
| MOTA | 398 | CZ | | | 50 | | 47.211 | | | | 7 6 |
| ATOM | 399 | CE | | | 50 | | 48.249 | | 53.318 | | 6 |
| ATOM | 400 |) C(| 3 ARG | A . | 50 | | 47.687 | | 54.172 | | 6 |
| ATOM | 401 | . CI | ARG | Α ! | 50 | | 48.818 | | 54.890 | | 6 |
| ATOM. | 402 | NE | E ARG | A ! | 50 | | 48.359 | | 55.762 | | . 7 |
| MOTA | 403 | CZ | Z ARG | Α : | 50 | | 47.708 | | 55.345 | | 6 |
| ATOM | 404 | NI: | 11 ARG | A : | 50 | | 47.430 | | 54.055 | 1.00 17.77 | 7 |
| ATOM | 405 | NH | 12 ARG | A ! | 50 | | 47.334 | | | | 7 |
| MOTA | 406 | C | _ARG | A ! | 50 | | 46.370 | | 51.723 | | 6 |
| MOTA | 407 | 0 | ARG | Α : | 0 | | 45.319 | | 52.206 | | 8 |
| MOTA | 408 | N | PRO | A 5 | 61 | | 46.823 | | 50.534 | | 7 |
| ATOM | 409 | CD | PRO | A 5 | 1 | • | 48.021 | | 49.789 | | 6 |
| ATOM | 410 | CA | PRO | A 5 | 1 | | 46.086 | | 49.761 | | 6 |
| MOTA | 411 | | PRO | A 5 | 1 | | 46.862 | 32.592 | 48.451 | | 6 |
| MOTA | 412 | | | | 1 | | 47.503 | 33.984 | 48.392 | | 6 |
| ATOM | 413 | C | PRO | A 5 | 1 | | 46.153 | 31.300 | 50.498 | 1.00 26.71 | 6 |
| ATOM | 414 | 0 | PRO | | 1 | | 47.071 | 31.066 | 51.293 | 1.00 31.32 | 8 |
| ATOM | 415 | N | ALA | | 2 | | 45.176 | 30.435 | 50.250 | 1.00 26.02 | 7 |
| ATOM | 416 | CA | | | 2 | • | 45.151 | 29.121 | 50.876 | 1.00 25.76 | 6 |
| ATOM | 417 | CB | | | 2 | | 43.720 | 28.585 | 50.933 | 1.00 21.42 | 6 |
| ATOM | 418 | C | ALA | | 2 | | 46.013 | 28.227 | 50.000 | 1.00 26.31 | 6 |
| ATOM | 419 | 0 | ALA | | 2 | | 45.878 | 28.239 | 48.780 | 1.00 30.31 | . 8 |
| ATOM | 420 | N | THR | | 3 | | 46.909 | 27.464 | 50.608 | 1.00 26.80 | 7 |
| ATOM | 421 422 | CA | | _ | | | 47.759 | 26.578 | 49.831 | 1.00 27.52 | 6 |
| ATOM ATOM | 423 | CB OG: | THR | | | | 48.845 | 25.975 | 50.717 | 1.00 26.27 | 6 |
| ATOM | 424 | CG | - | | | | 48.255 | 25.053 | 51.641 | 1.00 29.51 | 8 |
| ATOM | 425 | C C | THR | | | | 49.522 46.908 | 27.076 | 51.502 | 1.00 24.66 | 6 |
| MOTA | 426 | ō | THR | | | | 45.778 | 25.462 25.228 | 49.209 | 1.00 26.58 | 6 |
| ATOM | 427 | N | LYS | | | | 47.455 | 24.782 | 49.634 48.203 | 1.00 21.98 | 8 |
| ATOM | 428 | CA | LYS | | | | 46.739 | 23.713 | 47.507 | 1.00 29.62 1.00 32.62 | 7 |
| MOTA | 429 | CB | LYS | | | | 47.601 | 23.151 | 46.370 | 1.00 32.62 | 6 6 |
| ATOM | 430 | CG | LYS | A 5 | 4. | | 46.985 | 21.967 | 45.629 | 1.00 36.62 | 6 |
| MOTA | 431 | CD | LYS . | A 5 | 4 | | 45.733 | 22.352 | 44.866 | 1.00 40.69 | 6 |
| ATOM | 432 | CE | LYS . | A 5 | 1 | | 46.058 | 23.173 | 43.625 | | 6 |
| MOTA | 433 | NZ | LYS . | A 5 | 1 | | 46.844 | 22.393 | 42.614 | 1.00 50.68 | 7 |
| MOTA | 434 | C | LYS | | 1 | | 46.348 | 22.595 | 48.465 | 1.00 36.00 | 6 |
| ATOM | 435 | 0 | LYS | | | | 45.277 | 21.991 | 48.330 | 1.00 34.77 | 8 |
| ATOM | 436 | N | GLU | | | | 47.216 | 22.336 | 49.443 | 1.00 37.91 | 7 |
| ATOM | 437 | CA | GLU | | | | 46.979 | 21.290 | 50.433 | 1.00 36.96 | 6 |
| ATOM ATOM | 438 439 | CB CG | GLU 2 | | | | 48.240 | 21.100 | 51.281 | 1.00 40.29 | 6 |
| ATOM | 440 | CD | GLU A | | | | 48.216 | 19.887 | 52.195 | 1.00 47.95 | 6 |
| ATOM | 441 | OE1 | | | | | 49.552 49.659 | 19.654 | 52.891 | 1.00 51.01 | 6 |
| ATOM | 442 | OE2 | | | | | 50,497 | 18.688 20.437 | 53.679 | 1.00 52.65 | 8 |
| ATOM | 443 | c | GLU A | | | | 45.771 | 21.609 | 52.646 51.322 | 1.00 51.27 | 8 |
| ATOM - | 444 | ō | GLU A | | | • | 44.892 | 20.769 | 51.496 | 1.00 34.10 1.00 33.08 | 6 8 |
| ATOM | 445 | N | GLU A | | | | 45.723 | 22.827 | 51.866 | 1.00 33.08 | 7 |
| ATOM | 446 | CA | GLU A | | | | 44.621 | 23.256 | 52.733 | 1.00 32.39 | 6 |
| MOTA | 447 | CB. | GLU A | | | | 44.824 | 24.714 | 53.177 | 1.00 25.28 | 6 |
| ATOM | 448 | CG | GLU A | 56 | | | 46.204 | 24.994 | 53.758 | 1.00 28.82 | 6 |
| MOTA | 449 | CD | GLU A | 56 | | | 46.421 | 26.450 | 54.181 | 1.00 30.74 | 6 |
| MOTA | 450 | OE1 | GLU A | 56 | | | 46.072 | 27.369 | 53.398 | 1.00 29.77 | 8 |
| ATOM | 451 | OE2 | | | | | 46.969 | 26.674 | 55.288 | 1.00 25.98 | 8 |
| ATOM | 452 | C | GLU A | | | | 43.264 | 23.114 | 52.024 | 1.00 29.63 | 6 |
| ATOM | 453 | 0 | GLU A | | | | 42.299 | 22.584 | 52.595 | 1.00 29.90 | 8 |
| ATOM | 454 | N | LEU A | | | | 43.188 | 23.581 | 50.780 | 1.00 26.76 | 7 |
| ATOM | 455 | CA | LEU A | | | | 41.944 | 23.490 | 50.020 | 1.00 25.29 | 6 |
| ATOM | 456 | CB | LEU A | | | | 42.132 | 24.103 | 48.629 | 1.00 22.68 | 6 |
| ATOM | 457 | CG | LEU A | 57 | | | 42.402 | 25.612 | 48.572 | 1.00 22.39 | 5 |
| ATOM | 458 | CDI | LEU A | | | | 42.654 | 26.045 | 47.123 | 1.00 20.77 . | 6 |
| ATOM | 459 | | LEU A | 57 | | | 41.211 | 26.366 | 49.156 | 1.00 17.66 | 6 |
| ATOM | 460 | C | LEU A | 57 | | | 41.479 | 22.037 | 49.896 | 1.00 26.02 | 6 |
| | . 461 | N · | LEU A | 57 58 | | | 40.284 | 21.741 | 50.014 | 1.00 23.41 | 8 |
| ATOM | 462 | 14 | LEU A | | | | 42.444 | 21.143 | 49.675 | 1.00 24.82 | 7 |

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| ATOM | 46. | 3 CA | LE | TU A | A 58 | | 42.194 | 19.718 | 49.526 | 1.00 22.44 | 6 |
|--------------|------------|---------|------------|------------|----------|----|------------------|-------------------------------|------------------|--------------------------|--------|
| ATOM | 464 | 4 CB | L | U J | ¥ 58 | | 43.434 | 19.027 | 48.965 | 1.00 21.02 | 6 |
| ATOM | 469 | 5 CG | LE | EU J | ¥ 58 | | 43.838 | | | 1.00 22.94 | 6 |
| ATOM | 466 | 5 CD | 1 LE | U A | ¥ 58 | | 45.212 | | | 1.00 20.35 | 6 |
| ATOM | 467 | | 2 LE | U A | ¥ 58 | | 42.755 | 19.033 | | 1.00 23.28 | 6 |
| MOTA | 468 | 3 C | LE | TU P | 58 | | 41.797 | 19.054 | | 1.00 25.20 | Ğ |
| MOTA | 469 | | LE | U | 58 | | 41.456 | 17.867 | | 1.00 26.55 | 8 |
| ATOM | 470 | | | UA | - | | 41.858 | 19.794 | 51.938 | 1.00 25.44 | 7 |
| ATOM | 471 | | | U | | | 41.446 | 19.212 | 53.211 | 1.00 25.24 | 6 |
| ATOM | 472 | | | UA | | | 41.559 | | | 1.00 24.68 | 6 |
| ATOM | 473 | | | U A | | | 42.956 | | 54.912 | 1.00 27.05 | 6 |
| MOTA | 474 | | l LE | - | | | 42.912 | | 56.001 | 1.00 24.76 | . 6 |
| MOTA | 475 | | 2 LE | | | | 43.492 | | 55.474 | 1.00 26.99 | 6 |
| ATOM ATOM | · 476 | | | UA | | | 39.991 | | 53.045 | 1.00 24.22 | 6 |
| ATOM | 478 | | | UA | | | 39.548 | | 53.581 | 1.00 21.18 | 8 |
| ATOM | 479 | | | E A E A | | | 39.270 | | 52.270 | 1.00 25.00 | 7 |
| ATOM | 480 | | | E A | | | 37.859 37.054 | | 52.011 | 1.00 25.00 | 6 |
| ATOM | 481 | CG | | ΞA | | | 35.600 | 20.560 20.555 | 52.605 | 1.00 26.34 | 6 |
| ATOM | 482 | | L PH | | | | 34.811 | 19.422 | 52.223 52.427 | 1.00 29.37 | 6 |
| ATOM | 483 | | PH | | 60 | | 35.015 | 21.692 | 51.661 | 1.00 27.57 | 6 |
| ATOM | 484 | | PH | | 60 | | 33.466 | 19.419 | 52.077 | 1.00 27.33 1.00 27.00 | 6 |
| ATOM | 485 | CE2 | | ΕA | 60 | | 33.670 | 21.699 | 51.306 | 1.00 27.00 | 6 6 |
| ATOM | 486 | CZ | PH | EΑ | 60 | | 32.893 | 20.559 | 51.513 | 1.00 29.48 | 6 |
| ATOM | 487 | С | PHI | EΑ | 60 | | 37.506 | 19.214 | 50.538 | 1.00 27.78 | 6 |
| ATOM | 488 | 0 | | EΑ | 60 | | 37.022 | 18.143 | 50.158 | 1.00 31.57 | . 8 |
| ATOM | 489 | N | | 5 A | 61 | | 37.734 | 20.220 | 49.696 | 1.00 26.76 | 7 |
| ATOM | 490 | CA | | S A | 61 | | 37.376 | 20.056 | 48.287 | 1.00 28.84 | 6 |
| MOTA | 491 | CB | | 5 A | 61 | | 37.365 | 21.405 | 47.561 | 1.00 27.76 | 6 |
| MOTA MOTA | 492 493 | CCC | HIS | S A | 61 | | 36.385 | 22.396 | 48.117 | 1.00 30.54 | 6 |
| ATOM | 494 | | HIS | | 61 61 | | 35.056 | 22.549 | 47.907 | 1.00 33.74 | 6 |
| ATOM | 495 | | HIS | | 61. | | 36.750 35.691 | 23.401 | 48.987 | 1.00 34.02 | 7 |
| ATOM | 496 | | HIS | | 61 | | 34.649 | 24.135 _. 23.638 | | 1.00 32.07 | 6 |
| MOTA | 497 | c | HIS | | 61 | | 38.278 | 19.056 | 48.644 47.539 | 1.00 34.10 | 7 |
| ATOM | 498 | 0 | HIS | | 61 | | 39.287 | 18.604 | 48.072 | 1.00 28.38 1.00 25.81 | 6 8 |
| ATOM | 499 | N | THE | A | 62 | | 37.895 | 18.705 | 46.310 | 1.00 32.88 | 7 |
| ATOM | 500 | CA | THE | | 62 | | 38.658 | 17.749 | 45.488 | 1.00 34.68 | 6 |
| ATOM | 501 | CB | THE | | 62 | | 37.715 | 16.739 | 44.778 | 1.00 34.36 | 6 |
| MOTA | 502 | | THR | | 62 | | 36.942 | 17.415 | 43.778 | 1.00 34.81 | 8 |
| ATOM | 503 | | THR | | 62 | | 36.759 | 16.112 | 45.778 | 1.00 34.33 | 6 |
| MOTA | 504 | C | THR | | 62 | | 39.485 | 18.454 | 44.408 | 1.00 35.60 | 6 |
| ATOM | 505 506 | 0 | THR | | 62 | | 39.017 | 19.418 | 43.790 | 1.00 30.85 | 8 |
| ATOM ATOM | 507 | N CA | GLU | | 63 63 | | 40.700 | 17.958 | 44.166 | 1.00 37.38 | 7 |
| ATOM | 508 | CB | GLU | | 63 | | 41.587 42.759 | 18.555 | 43.165 | 1.00 40.68 | 6 |
| ATOM | 509 | CG | GLU | | 63 | | 43.719 | 17.626 17.389 | 42.840 43.987 | 1.00 43.75 1.00 50.68 | 6 |
| ATOM | 510 | CD | GLU | | 63 | | 45.026 | 16.760 | 43.529 | 1.00 50.68 1.00 55.36 | 6 |
| ATOM | 511 | OE1 | GLU | A | 63 | | 45.789 | 17.441 | 42.808 | 1.00 53.03 | 6 8 |
| ATOM | 512 | OE2 | GLU | Α | 63 | | 45.285 | 15.585 | 43.883 | 1.00 59.56 | 8 |
| ATOM | 513 | С | GLU | A | 63 | | 40.894 | 18.939 | 41.860 | 1.00 39.26 | 6 |
| MOTA | 514 | 0 | GLU | A | 63 | | 40.771 | 20.116 | 41.535 | .1.00 42.33 | 8 |
| ATOM | 515 | N | ASP | | 64 | | 40.453 | 17.948 | 41.102 | 1.00 37.07 | 7 |
| MOTA | 516 | CA | ASP | | 64 | | 39.782 | 18.224 | 39.845 | 1.00 36.98 | 6 |
| ATOM | 517 | CB | ASP | | 64 | | 38.957 | 17.000 | 39.426 | 1.00 42.19 | 6 |
| ATOM | 518 | CG | ASP | | 64 | | 38.037 | 16.501 | 40.533 | 1.00 47.66 | 6 |
| ATOM | 519 | OD1 | | | 64 | | 37.039 | 17.193 | 40.851 | 1.00 47.95 | 8 |
| ATOM | 520 | OD2 | | | 64 | | 38.325 | 15.413 | 41.091 | 1.00 50.07 | 8 |
| MOTA | 521 | | ASP | | 64 | | 38.908 | 19.480 | 39.906 | 1.00 33.40 | 6 |
| ATOM | 522 523 | | ASP | | 64 55 | | 38.927 | 20.293 | 38.986 | 1.00 33.64 | 8 |
| ATOM ATOM | 524 | | TYR TYR | | 65 65 | | 38.156 | 19.641 | 40.990 | 1.00 30.57 | 7 |
| MOTA MOTA | 525 | | TYR | | 65 | | 37.286 | 20.806 | 41.157 | 1.00 29.65 | 6 |
| atom atom | 526 | | TYR | | 65 | | 36.300 35.557 | 20.560 | 42.316 | 1.00 30.16 | 6 |
| ATOM | 527 | CD1 | | | 65 | | 34.791 | 21.790 22.572 | 42.810 41.944 | 1.00 28.49 1.00 30.25 | 6 6 |
| ATOM | 528 | CEI | | | 65 | ٠. | 34.126 | 23.715 | 42.399 | 1.00 30.25 | 6. |
| | | | , | - | - | | | 20.120 | | 2.00 20.30 | - |

| ATOM | 529 CD2 TYR A 65 | 35.638 | 2 22 201 44 | |
|--------|------------------|----------------|-------------|--------------------|
| ATOM | | | | 1.150 1.00 28.28 6 |
| | | 34.980 | 0 23.320 44 | 1.617 1.00 26.96 6 |
| ATOM | 531 CZ TYR A 65 | 34.227 | | |
| ATOM | 532 OH TYR A 65 | 33.568 | | |
| | | | | .207 1.00 28.53 g |
| ATOM | | 38.118 | 3 22.061 41 | .418 1.00 29.15 6 |
| MOTA | 534 O TYR A 65 | 37.860 | | |
| ATOM | 535 N ILE A 66 | | | |
| | | 39.122 | | .270 1.00 26.61 7 |
| ATOM | 536 CA ILE A 66 | 39.986 | 23.041 42 | |
| ATOM | 537 CB ILE A 66 | 40.998 | | 600 |
| ATOM | | | | .687 1.00 26.25 6 |
| | | 42.009 | 23.753 43 | .869 1.00 21.20 6 |
| MOTA | 539 CG1 ILE A 66 | 40.264 | 22.341 44 | |
| ATOM | 540 CD1 ILE A 66 | 39.478 | | |
| ATOM | | | | .555 1.00 30.52 6 |
| | | 40.761 | 23.504 41 | .381 1.00 28.07 6 |
| ATOM | 542 O ILE A 66 | 41.039 | | 205 4 24 |
| ATOM | 543 N ASNA 67 | 41.125 | | |
| ATOM | | | | .521 1.00 28.47 7 |
| | 544 CA ASN A 67 | 41.902 | 22.898 39 | .337 1.00 30.15 6 |
| MOTA | 545 CB ASN A 67 | 42.563 | 21.656 38 | |
| MOTA | 546 CG ASN A 67 | | | |
| | | 43.712 | | .578 1.00 38.78 6 |
| MOTA | 547 OD1 ASN A 67 | 44.674 | 21.841 39 | .878 1.00 43.34 8 |
| MOTA | 548 ND2 ASN A 67 | 43.626 | | .956 1.00 37.14 7 |
| ATOM | 549 C ASN A 67 | | | , |
| | | 41.020 | | .314 1.00 28.41 6 |
| MOTA | 550 O ASN A 67 | 41.494 | 24.354 37 | .499 1.00 28.05 8 |
| ATOM | 551 N THRA 68 | 39.733 | | |
| ATOM | 552 CA THR A 68 | | | |
| | | 38.787 | 23.791 37 | .416 1.00 21.75 6 |
| ATOM | 553 CB THR A 68 | 37.438 | 23.111 37 | .500 1.00 16.99 6 |
| ATOM | 554 OG1 THR A 68 | 37.620 | | |
| ATOM | 555 CG2 THR A 68 | 36.549 | | 200 |
| ATOM | | | | .359 1.00 17.59 6 |
| | | 38.633 | 25.263 37. | 732 1.00 22.13 6 |
| MOTA | 557 O THRA 68 | 38.529 | 26.088 36. | |
| ATOM | 558 N LEUA 69 | 38.645 | | |
| ATOM | | | | .023 1.00 22.32 7 |
| | | 38.535 | 26.956 39. | 482 1.00 23.97 6 |
| ATOM | 560 CB LEU A 69 | 38.376 | 26.982 41. | 000 1.00 24.99 6 |
| ATOM | 561 CG LEU A 69 | 37.023 | | 540 1 00 00 00 |
| MOTA | | | | 548 1.00 29.08 6 |
| | F 53 | 37.08 7 | 26.416 43. | 066 1.00 30.99 6 |
| ATOM | 563 CD2 LEU A 69 | 35.942 | 27.528 41. | 120 1.00 28.69 6 |
| MOTA | 564 C LEUA 69 | 39.772 | | |
| ATOM | 565 O LEU A 69 | | | |
| | | 39.683 | | 674 1.00 25.04 8 |
| ATOM | 566 N MET A 70 | 40.932 | 27.128 39. | 218 1.00 24.67 7 |
| MOTA | 567 CA MET A 70 | 42.183 | | |
| ATOM | 568 CB MET A 70 | 43.358 | | - |
| ATOM | | | | 380 1.00 26.92 6 |
| | | 43.418 | 26.751 40. | 884 1.00 26.69 6 |
| ATOM | 570 SD MET A 70 | 44.970 | 25.929 41. | 325 1.00 30.71 16 |
| ATOM | 571 CE MET A 70 | 46.137 | | |
| ATOM | 572 C MET A 70 | | | 642 1.00 23.20 6 |
| | | 42.324 | | 412 1.00 21.62 6 |
| ATOM | 573 O MET A 70 | 42.903 | 29.041 36. | 982 1.00 18.99 8 |
| MOTA | 574 N GLUA 71 | 41.769 | 27.122 3€ | |
| ATOM | 575 CA GLU A 71 | | | |
| ATOM | | 41.859 | 27.204 35. | |
| | | 41.681 | 25.814 34 | 582 1.00 26.22 6 |
| ATOM | 577 CG GLU A 71 | 42.224 | 25.695 33. | |
| ATOM | 578 CD GLU A 71 | 43.737 | | |
| ATOM | | | | |
| | | 44.288 | 25.855 31. | 983 1.00 35.84 8 |
| ATOM | 580 OE2 GLU A 71 | 44.377 | 26.116 34. | 154 1.00 30.13 8 |
| ATOM | 581 C GLU A 71 | 40.845 | | |
| ATOM | | | | |
| | | 41.144 | 28.851 33.0 | 626 1.00 21.54 8 |
| ATOM | 583 N ALA A 72 | 39.649 | 28.197 35.3 | |
| ATOM | 584 CA ALA A 72 | 38.589 | | |
| | | | 29.067 34. | |
| MOTA | 585 CB ALA A 72 | 37.298 | 28.743 35.3 | 397 1.00 19.23 6 |
| ATOM | 586 C ALA A 72 | 38.931 | 30.536 34.8 | |
| ATOM | 587 O ALA A 72 | 38.711 | 21 202 34 4 | |
| | | | 31.383 34.0 | |
| MOTA | 588 N GLU A 73 | 39.470 | 30.835 36.0 | |
| ATOM | 589 CA GLUA 73 | 39.820 | 32.202 36.4 | 436 1.00 29.44 6 |
| MOTA | 590 CB GLU A 73 | 40.157 | 32.282 37.9 | |
| ATOM | | | 24.404 31.3 | |
| | | 40.646 | 33.655 38.3 | |
| ATOM . | 592 CD GLU A 73 | 40.840 | 33.806 39.8 | |
| ATOM | 593 OE1 GLU A 73 | 39.841 | 33.776 40.5 | |
| ATOM | 594 OE2 GLU A 73 | 41.996 | | |
| ATOM. | | 41.230 | 33.960 40.2 | 277 1.00 31.77 8 |
| • | | | - | |

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| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 595 596 597 598 599 600 601 602 603 604 605 606 | NH: C O | ARG ARG | A A A A A A A A A A A A A A A A A A A | 73 74 74 74 74 74 74 74 74 | 40.946 40.859 41.992 43.128 44.405 44.514 45.702 46.041 46.646 46.989 46.906 42.894 | 33.465 | 35.615 35.259 35.309 34.557 34.874 34.205 34.754 33.933 32.748 32.232 32.079 33.051 32.338 | 1.00 31.83 1.00 33.52 1.00 31.45 1.00 30.65 1.00 32.12 1.00 31.42 1.00 34.18 1.00 35.55 1.00 29.64 1.00 34.07 1.00 28.61 1.00 24.38 | 6 8 7 6 6 6 6 7 6 7 6 8 |
|--|--|---------------|------------|---|--|--|------------------|--|--|--|
| MOTA | 608 609 | N | CYS | | 75 75 | 42.107 | 31.673 | 32.566 | 1.00 28.32 | 7 |
| ATOM ATOM | 610 | CA CB | CA2. | | 75 | 41.796 41.687 | 31.619 30.167 | 31.148 30.682 | 1.00 32.42 1.00 32.91 | 6 6 |
| MOTA | 611 | SG | CYS | | 75 | 43.281 | 29.296 | 30.777 | 1.00 37.09 | 16 |
| ATOM | 612 | С | CYS | A | 75 | 40.489 | 32.382 | 30.956 | 1.00 33.10 | 6 |
| MOTA | 613 | 0 | CYS | | 75 | 40.029 | 32.598 | 29.834 | 1.00 30.74 | 8 |
| MOTA | 614 | N | GLN | | 76 | 39.914 | 32.787 | 32.088 | 1.00 34.42 | 7 |
| ATOM ATOM | 61,5 61.6 | CA CB | GLN GLN | | 76 76 | 38.691 38.986 | 33.575 34.962 | 32.144 31.578 | 1.00 33.20 1.00 32.09 | 6 6 |
| MOTA | 617 | CG | GLN | | 76 | 38.089 | 36.064 | 32.094 | 1.00 32.09 | 6 |
| ATOM | 618 | CD | GLN | | 76 | 38.479 | 36.541 | 33.480 | 1.00 41.47 | 6 |
| ATOM | 619 | OE1 | | | 76 | 38.574 | 35.755 | 34.426 | 1.00 45.02 | `8 |
| ATOM | 620 | NE2 | | | 76 | 38.703 | 37.846 | 33.606 | 1.00 42.22 | 7 |
| ATOM ATOM | 621 622 | C O | GLN GLN | | 76 76 | 37.561 36.732 | 32.920 33.598 | 31.358 30.760 | 1.00 33.20 1.00 34.19 | 6 8 |
| MOTA | 623 | N | CYS | | 7 7 | 37.522 | 31.598 | 31.370 | 1.00 31.81 | 7 |
| MOTA | 624 | CA | CYS | | 77 | 36.511 | 30.862 | 30.627 | 1.00 31.47 | 6 |
| MOTA | 625 | CB | CYS | | 77 | 37.187 | 30.181 | 29.454 | 1.00 30.25 | 6 |
| MOTA MOTA | 626 627 | SG C | CYS | | 77. 7 7 | 38.479 35.851 | 29.071 29.795 | 30.044 31.498 | 1.00 33.94 1.00 31.97 | 16 |
| MOTA | 628 | Ö | CYS | | 77 | 36.335 | 29.503 | 32.590 | 1.00 31.97 | 6 8 |
| ATOM | 629 | N | VAL | | 78 | 34.750 | 29.216 | 31.018 | 1.00 30.78 | 7 |
| ATOM | 630 | CA | VAL | | 78 | 34.069 | 28.139 | 31.747 | 1.00 30.55 | 6 |
| ATOM | 631 632 | CB | VAL VAL | | 78 78 | 32.539 | 28.287 | 31.720 | 1.00 30.06 | 6 |
| ATOM ATOM | 633 | | VAL | | 78 | 31.881 32.129 | 27.030 29.503 | 32.293 32.526 | 1.00 28.23 | 6 6 |
| ATOM | 634 | C | VAL | | 78 | 34.420 | 26.794 | 31.110 | 1.00 29.80 | 6 |
| MOTA | 635 | 0 | VAL | | 78 | 33.851 | 26.422 | 30.077 | 1.00 29.65 | 8 |
| ATOM | 636 | N | | | 79 | 35.337 | 26.033 | 31.739 | 1.00 28.55 | 7 |
| ATOM ATOM | 637 638 | CD | PRO PRO | | 79 79 | 35.985 35.793 | 26.335 24.724 | 33.025 31.261 | 1.00 24.39 | 6 6 |
| ATOM | 639 | CB | PRO | | 79 | 36.622 | 24.218 | 32.434 | 1.00 24.49 | 6 |
| ATOM | 6.0 | CG | PRO | | 79 | 37.239 | 25.500 | 32.922 | 1.00 25.68 | 6 |
| MOTA | 61 | С | PRO | | 79 | 34.668 | 23.776 | 30.881 | 1.00 30.13 | 6 |
| MOTA | 6 ₃ 2 643 | N O | PRO LYS | | 79 | 33.697 | 23.624 | 31.615 29.727 | 1.00 30.87 | 8 |
| MOTA MOTA | 644 | CA | LYS | | 80 80 | 34.796 33.758 | 23.136 22.216 | 29.727 | 1.00 33.44 1.00 38.52 | 7 6 |
| ATOM | 645 | CB | LYS | | 80 | 34.202 | 21.421 | 28.076 | 1.00 45.18 | 6 |
| MOTA | 646 | CG | LYS | | 80 | 35.450 | 20.589 | 28.278 | 1.00 55.18 | 6 |
| MOTA | 647 | CD | LYS | | 30 | 35.788 | 19.827 | 27.000 | 1.00 60.80 | 5 |
| ATOM | . 648 | CE NZ | LYS . | | 30 | 37.035 37.367 | 18.976 | 27.168 | 1.00 64.25 | 6 |
| ATOM ATOM | 649 650 | C | LYS | | 30 30 | 33.411 | 18.252 21.267 | 25.911 30.443 | 1.00 68.95 1.00 36.56 | 7 6 |
| ATOM | 651 | ō | LYS | | 30 | 34.293 | 20.775 | 31.164 | 1.00 31.61 | 8 |
| ATOM | 652 | N | GLY . | | 31 | 32.112 | 21.035 | 30.602 | 1.00 32.57 | 7 |
| ATOM | 653 | CA | GLY . | | 31 | 31.634 | 20.155 | 31.648 | 1.00 29.81 | 6 |
| ATOM | 654 655 | C | GLY . | | 31 | 31.477 30.544 | 20.884 | 32.965 33.723 | 1.00 28.30 | 6 8 |
| ATOM ATOM | 655 656 | O N | ALA. | | 31 32 | 30.344 | 20.612 21.830 | 33.723 | 1.00 25.49 | 7 |
| ATOM | 657 | CA | ALA | | 32 | 32.384 | 22.602 | 34.458 | 1.00 26.72 | 6 |
| ATOM | 658 | CB | ALA | 3 A | 32 | 33.485 | 23.674 | 34.406 | 1.00 22.64 | 6 |
| ATOM | 659 | C | ALA | | 32 | 31.066 | 23.245 | 34.886 | 1.00 27.84 | 6 |
| ATOM | 660 | 0 . | ALA A | A . | 32 | 30.729 | 23.224 | 36.068 | 1.00 30.00 | 8 |

| ATOM | 661 N ARG A 83 | 20 210 02 044 | |
|--------|--|--|-----|
| MOTA | CC0 01 11.01. | 30.310 23.811 33.951 1.00 31.15 | 7 |
| | | 29.071 24.462 34.345 1.00 32.50 | |
| MOTA | 663 CB ARG A 83 | 22 22 21 21 21 21 21 21 21 21 21 21 21 2 | 6 |
| ATOM | CCA 50 | | 6 |
| | CCE 05 | 47.439 26.189 33.408 1.00 42 23 | 6 |
| MOTA | 665 CD ARG A 83 | | |
| ATOM- | 666 NE ARG A 83 | 25 204 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 | 6 |
| ATOM | CCD 00 | 34.330 2.00 31.00 | 7 |
| | ·;= •• • • • • • • • • • • • • • • • • • | 25.046 27.460 36.005 1.00 56.84 | |
| ATOM | 668 NH1 ARG A 83 | 2.00 20.04 | 6 |
| ATOM | | 24 500 33.05 | 7 |
| | 05 | 24.588 28.672 36.304 1.00 58.03 | 7 |
| atom | 670 C -ARG A 83 | | |
| ATOM | 671 O ARG A 83 | 20 055 | 6 |
| ATOM | C70 19 000 | 23.67 | 8 |
| | | 27.648 22.491 34.581 1.00 33.06 | 7 |
| MOTA | 673 CA GLUA 94 | | |
| ATOM | 674 CB GLU A 84 | 1.00 35.40 | 6 |
| ATOM | | 26.112 20.562 34.417 1.00 37.35 | . 6 |
| | | 26.989 19.684 33.496 1.00 40.01 | |
| ATOM | 676 CD GLUA 84 | 2.00 40.01 | 6 |
| ATOM | 677 OE1 GLU A 84 | 27 225 42 | 6 |
| | 570 000 000 7 04 | 27.925 19.723 31.292 1.00 41.12 | 8 |
| ATOM | 678 OE2 GLU A 84 | 27.636 21.671 32.270 1.00 41.01 | |
| MOTA | 679 C GLUA 84 | 27 617 | 8 |
| ATOM | COO - | 20.21, 1.00 35.42 | 6 |
| | CO4 | 27.246 20.816 37.594 1.00 34 66 | 8 |
| MOTA | 681 N LYS A 85 | 28.727 20.226 36.002 1.00 35 21 | |
| ATOM | 682 CA LYS A 85 | 30.502 1.00 33.21 | 7 |
| ATOM | 600 | 20 37.93 | 6 |
| | COA | 30.841 19.030 36.076 1.00 40.61 | 6 |
| atom | 684 CG LYS A 85 | 2 | |
| ATOM | 685 CD LYS A 85 | 2.00 42.63 | 6 |
| ATOM | | 31.038 16.640 36.872 1.00 45.48 | 6 |
| | COS | 32.034 15.523 37.078 1 00 45 60 | 6 |
| atom | 687 NZ LYS A 85 | 33.032 15.833 38.154 1.00 46.16 | |
| ATOM | 688 C LYS A 85 | 1.00 40.10 | 7 |
| ATOM | | 37.36 | 6 |
| | COO 12 12 00 | 30.161 19.516 39.222 1.00 38.40 | a |
| MOTA | 690 N TYRA 86 | | |
| ATOM | 691 CA TYR A 86 | | 7 |
| ATOM | COO OD | 25 12 12 12 12 12 12 12 12 12 12 12 12 12 | 6 |
| | (0) | 32.151 22.610 39.200 1.00 32.09 | 6 |
| MOTA | 693 CG TYR A 86 | | |
| MOTA | 694 CD1 TYR A 86 | 23 120 20 20 20 20 20 20 20 20 20 20 20 20 2 | б |
| ATOM | | 1.00 32.12 | 6 |
| | 695 CEI TYR A 86 | 33.918 19.266 39.723 1.00 33.59 | 6 |
| MOTA | 696 CD2 TYR A 86 | 33.839 21.306 37.841 1.00 33.82 | |
| ATOM | 697 CE2 TYR A 86 | 34 545 55 55 | 6 |
| ATOM | | 1.00 34,35 | 6 |
| | | 34.675 19.162 38.566 1.00 32.38 | 6 |
| ATOM | 699 OH TYR A 86 | 35.431 18.034 38.336 1.00 29.17 | |
| MOTA | 700 C TYR A 86 | 1,00 29,17 | 8 |
| ATOM | 701 O TYR A 86 | 1.00 50.21 | 6 |
| ATOM | 700 | 30.192 24.265 40.445 1.00 29.12 | 8 |
| | 702 N ASNA 87 | 28.712 23.594 38.893 1.00 29.44 | 7 |
| ATOM | 703 CA ASN A 87 | | |
| ATOM | 704 CB ASN A 87 | 27 154 24 610 | 6 |
| ATOM | | 27.154 24.618 40.470 1.00 25.63 | 6 |
| | | 25.871 25.428 40.596 1.00 28.05 | 6 |
| ATOM | 706 OD1 ASN A 87 | 25 255 25 | |
| ATOM | 707 ND2 ASN A 87 | 32:072 1:00 1:32 | 8 |
| ATOM | | | 7 |
| | 500 - | 28.580 26.015 38.963 1.00 1.35 | 6 |
| ATOM | 709 O ASNA 87 | | |
| ATOM | 710 N ILE A 88 | 20 545 | . 8 |
| ATOM | | | 7 |
| | 740 | 30.407 27.173 37.809 1.00 33.77 | 6 |
| MOTA | 712 CB ILE A 88 | 31.894 26.734 37.776 1.00 36.13 | |
| ATOM | 713 CG2 ILE A 88 | | 6 |
| ATOM | | 2.00 37.80 | 6 |
| | | 32.357 26.342 39.178 1.00 38.92 | 6 |
| ATOM . | 715 CD1 ILE A 88 | 32.350 27.483 40.176 1.00 41.44 | |
| ATOM | 716 C ILE A 88 | | 6 |
| ATCM | | 20 722 | 6 |
| | | 29.708 27.196 35.520 1.00 32 72 | 8 |
| ATOM | 718 N GLY A 89 | 30.237 29.179 36.438 1.00 31.56 | |
| ATOM | 719 CA GLY A 89 | | 7 |
| ATOM | | 200 30.04 | 6 |
| | | 28.696 30.689 35.093 1.00 32.17 | 6 |
| ATOM | 721 O GLY A 89 | 28.628 31.670 34.349 1.00 30.42 | |
| ATOM | 722 N GLY A 90 | | 8 |
| ATOM | | 26 302 | 7 |
| | | 26.387 30.937 35.756 1.00 32.92 | 5 |
| atom · | 724 C GLY A 90 | 26.316 32.246 36.524 1.00 34.32 | 6 |
| ATCM | 725 O GLY A 90 | | |
| ATOM | | | 8 |
| | 726 N TYR A 91 | 25.144 32.882 36.504 1.00 33.88 | 7 |
| | • | • | |

| MOTA | 727 | CA TYR | A 91 | 24.924 | 34.146 | 37.206 | 1 00 25 76 | _ |
|--------|-------------|-----------|----------|----------|----------|--------|------------|-----|
| MOTA | 728 | CB TYR | | 23.46 | | | | 6 |
| ATOM | 729 | CG TYR | | 23.089 | | | | 6 |
| ATOM | 730 | CD1 TYR | | | | 37.990 | | 6 |
| | | | | 23.417 | | 37.688 | 1.00 43.57 | 6 |
| MOTA | 731 | CE1 TYR | | 23.105 | | 38.577 | | 5 |
| MOTA | 732 | CD2 TYR | | 22.444 | 35.484 | 39.205 | | |
| MOTA | 733 | CE2 TYR | A 91 | 22.132 | | 40.097 | | 6 |
| MOTA | 734 | CZ TYR | | 22.462 | | 30.097 | 1.00 42.67 | 6 |
| ATOM | 735 | OH TYR | | | | 39.775 | 1.00 42.41 | 6 |
| | | | | 22.130 | 38.835 | 40.646 | 1.00 43.69 | 8 |
| MOTA | 736 | C TYR | | 25.242 | 34.082 | 38.701 | 1.00 34.15 | 6 |
| MOTA | 737 | O TYR | A 91 | 25.821 | 35.014 | 39.266 | 1.00 29.52 | 8 |
| ATOM | 738 | N GLU | A 92 | 24.837 | | 39.333 | | |
| ATOM | 739 | CA GLU | | 25.024 | | | 1.00 34.78 | 7 |
| MOTA | 740 | CB GLU | | | | 40.767 | 1.00 38.46 | 6 |
| ATOM | 741 | | | 24.233 | | 41.211 | 1.00 43.99 | 6 |
| | | | | 23.932 | | 42.700 | 1.00 52.10 | . 6 |
| ATOM | 742 | CD GLU | | 23.294 | 30.161 | 43.097 | 1.00 58.00 | 6 |
| MOTA | 743 | OE1 GLU | A 92 | 24.001 | 29.126 | 43.058 | 1.00 60.63 | |
| ATOM | 744 | OE2 GLU | A 92 | . 22.087 | 30.149 | 43.434 | 1.00 59.58 | 8 |
| ATOM | 745 | C GLU | A 92 | 26.492 | 32.669 | | | 8 |
| ATOM | 746 | O GLU | | | | 41.208 | 1.00 36.42 | 5 |
| ATOM | 747 | N ASN | | 26.902 | 33.287 | 42.193 | 1.00 32.92 | 8 |
| | | | | 27.280 | 31.883 | 40.473 | 1.00 34.12 | 7 |
| ATOM | 748 | CA ASN | | 28.693 | 31.671 | 40.808 | 1.00 33.24 | 6 |
| ATOM | 749 | CB ASN . | A 93 | 28.871 | 30.259 | 41.364 | 1.00 28.52 | 6 |
| ATOM . | 750 | CG ASN | A 93 | 27.734 | 29.859 | 42.299 | 1.00 27.45 | |
| MOTA | 751 | OD1 ASN | A 93 | 27.547 | 30.457 | 43.355 | 1.00 27.45 | 6 |
| ATOM | 752 | ND2 ASN | | 26.956 | | | 1.00 21.76 | 8 |
| ATOM | 753 | C ASN | | | . 28.853 | 41.895 | 1.00 21.79 | 7 |
| MOTA | 754 | | | 29.529 | 31.843 | 39.535 | 1.00 35.04 | 6 |
| | | | | 30.160 | 30.898 | 39.059 | 1.00 33.81 | 8 |
| ATOM | 755 | N PRO | | 29.583 | 33.081 | 39.010 | 1.00 36.19 | 7 |
| MOTA | 756 | CD PRO | A 94 | 28.970 | 34.231 | 39.690 | 1.00 34.62 | 6 |
| MOTA | 757 | CA PRO | 94 | 30.274 | 33.560 | 37.808 | 1.00 34.80 | 6 |
| ATOM | 758 | CB PRO A | A 94 | 29.924 | 35.050 | 37.791 | | |
| ATOM | 75 <i>9</i> | CG PRO A | | 28.619 | 35.095 | | 1.00 33.94 | 6 |
| ATOM | 760 | C PRO F | | | | 38.516 | 1.00 36.13 | 6 |
| | 761 | | | 31.775 | 33.379 | 37.733 | 1.00 34.63 | 6 |
| ATOM | | O PRO A | | 32.443 | 33.103 | 38.730 | 1.00 34.72 | 8 |
| ATOM | 762 | N VAL | | 32.299 | 33.556 | 36.526 | 1.00 33.57 | 7 |
| ATOM | 763 | CA VAL A | | 33.735 | 33.499 | 36.307 | 1.00 30.31 | 6 |
| ATOM | 764 | CB VAL A | 95 | 34.085 | 33.171 | 34.841 | 1.00 29.88 | 6 |
| ATOM | 765 | CG1 VAL A | 95 | 35.561 | 33.453 | 34.574 | · | |
| ATOM | 766 | CG2 VAL A | | 33.795 | 31.713 | | 1.00 29.53 | 6 |
| ATOM | | C VAL A | | | | 34.563 | 1.00 28.05 | 6 |
| ATOM | | O VAL A | | 34.195 | 34.910 | 36.624 | 1.00 29.86 | 6 |
| | | | | 33.524 | 35.879 | 36.272 | 1.00 29.07 | 8 |
| MOTA | | N SER A | | 35.318 | 35.019 | 37.317 | 1.00 30.89 | 7 |
| ATOM | | CA SERA | | 35.889 | 36.310 | 37.687 | 1.00 32.27 | 6 |
| MOTA | 771 | CB SER A | 96 | 34.885 | 37.145 | 38.501 | 1.00 30.16 | 6 |
| MOTA | 772 | OG SER A | 96 | 34.600 | 36.545 | 39.756 | 1.00 26.77 | |
| MOTA | 773 | C SER A | 96 | 37.111 | 35.993 | 38.537 | | 8 |
| MOTA | | O SER A | | 37.603 | | | 1.00 32.96 | 6 |
| ATOM | | _ | | | 34.865 | 38.511 | 1.00 33.77 | 8 |
| | | | | 37.609 | 36.973 | 39.282 | 1.00 32.66 | 7 |
| ATOM | | CA TYR A | 97 | 38.753 | 36.712 | 40.132 | 1.00 31.95 | 6 |
| MOTA | | CB TYR A | 97 | 39.838 | 37.766 | 39.923 | 1.00 31.81 | 6 |
| ATOM | 778 (| CG TYR A | 97 | 40.416 | 37.729 | 38.525 | 1.00 30.39 | 6 |
| MOTA | 779 (| CD1 TYR A | 97 | 39.820 | 38.434 | 37.479 | | |
| ATOM | | CE1 TYR A | 97 | | | 37.473 | 1.00 30.63 | 6 |
| | | D2 TYR A | | 40.327 | 38.358 | 36.178 | 1.00 28.49 | 6 |
| ATOM | | | 97 | 41.536 | 36.945 | 38.236 | 1.00 28.43 | 6 |
| ATOM | | E2 TYR A | 97 | 42.046 | 36.858 | 36.942 | 1.00 24.73 | 6 |
| ATOM | 783 C | Z TYR A | 97 | 41.437 | 37.565 | 35.919 | 1.00 27.27 | 6 |
| atom | 784 C | H TYR A | 97 | 41.915 | 37.455 | 34.633 | 1.00 26.70 | |
| ATOM | 785 C | | 97 | 38.350 | | | 1 00 21 10 | 8 |
| | 786 C | | | _ | 36.618 | 41.596 | 1.00 31.10 | 6 |
| MOTA | | | 97 00 | 39.178 | 36.735 | 42.495 | 1.00 33.01 | 8 |
| atom | 787 N | | 98 | 37.059 | 36.398 | 41.818 | 1.00 31.11 | 7 |
| ATOM | | A ALA A | 98 | 36.510 | 36.241 | 43.160 | 1.00 30.06 | 5 |
| MOTA | 789 C | B ALA A | 98 | 35.141 | 36.920 | 43.256 | 1.00 27.71 | 6 |
| ATCM | 790 C | | 98 | 36.350 | 34.736 | 43.357 | 1.00 31.24 | 6 |
| ATCM | 791 C | • | 98 | 36.335 | | | | |
| | 792 N | | 99 | | 34.238 | 44.487 | 1.00 29.66 | -8 |
| MOTA | , 32 IV | . ner w | | 36.249 | 34.030 | 42.230 | 1.00 29.50 | 7 |
| | | | | | | | | |

| ATOM | 1 793 CA MET A 99 | 76.040 | |
|---------|-------------------|--|----|
| ATOM | 4 704 05 | 36.048 32.589 42.207 1.00 29.89 | _ |
| ATOM | n JJ | | 6 |
| | | | 6 |
| ATOM | | 36 426 23 23 22 1.00 29.63 | 6 |
| MOTA | 797 CE MET A 99 | 35 630 55 30.120 1.00 29.78 | 16 |
| MOTA | | 33.023 30.2/3 38.347 1.00 25 05 | -6 |
| MOTA | 700 0 | 31.00U 47 793 7 00 30 5 | |
| | • • | | 6 |
| ATOM | | 30 417 30 100 1.00 30.59 | 8 |
| ATOM | 801 CA PHE A 100 | 20 554 11 12 12 13 13 13 13 13 13 13 13 13 13 13 13 13 | 7 |
| ATOM | 802 CB PHE A 100 | 43.114 1.00 33 87 | 6 |
| ATOM | 803 CG PHE A 100 | -0.022 JU.01/ 47 070 1 00 12 02 | |
| ATOM | | | 6 |
| | | 41 152 22 | 6 |
| MOTA | A 100 | 12 750 70 70 70 10 10 41.84 | 6 |
| ATOM | 806 CE1 PHE A 100 | 30.339 42.372 1.00 42 19 | 6 |
| ATOM | 807 CE2 PHE A 100 | ******* | |
| ATOM | 808 CZ PHE A 100 | 43.808 29.600 42 944 1 00 45 | 6 |
| | | 43 E13 35 100 40.50 | 6 |
| MOTA | 809 C PHE A 100 | 40 510 55 120 120 120 120 139.89 | 6 |
| MOTA | 810 O PHE A 100 | 40 706 33.98 | 6 |
| ATOM | 811 N THR A 101 | 32.231 45.088 1.00 38 21 | 8 |
| ATOM | | ****** 33.615 43 245 7 66 66 | |
| ATOM | | 42.063 34.261 43 969 1 00 00 00 | 7 |
| | 813 CB THR A 101 | 42 622 26 27 | б |
| ATOM | 814 OG1 THR A 101 | 43 444 5 1.00 22.48 | 6 |
| ATOM | 815 CG2 THR A 101 | 42 450 | 8 |
| ATOM | 816 C THR A 101 | 30.333 43.876 1.00 15 00 | 6 |
| ATOM | | 34.860 45.205 1 00 21 71 | |
| ATOM | | 41.988 34.845 46 282 1 00 22 | 6 |
| | 818 N GLY A 102 | 40 107 7 23.82 | 8 |
| ATOM | 819 CA GLY A 102 | 70 577 77 77 77 77 77 77 77 77 77 77 77 77 | 7 |
| ATOM | 820 C GLY A 102 | 30 000 21.23 | 6 |
| ATOM | 821 O GLY A 102 | 34.833 47.153 1.00 23 03 | 6 |
| ATOM | 822 N SER A 103 | 33.203 34.309 48.378 1 00 20 42 | |
| ATOM | | 70 610 70 70 70 70 70 70 70 | 8 |
| | 823 CA SER A 103 | 38.028 32.640 47.276 1.00 22.59 | 7 |
| ATOM | 824 CB SER A 103 | 37 464 37 270 1.00 20,51 | 6 |
| ATOM | 825 OG SER A 103 | 26 224 22 20 28 10 | 6 |
| ATOM | 826 C SER A 103 | 32.099, 45.639 1.00 32 01 | 8 |
| ATOM | | 32.400 32.040 48 N32 1 NN 22 32 | |
| ATOM | | 39.019 31.544 49 144 1 00 30 65 | 6 |
| | 828 N SER A 104 | 40.364 32 080 47 410 1 00 30.61 | 8 |
| ATOM | 829 CA SER A 104 | 41 500 21 - 1.00 48.70 | 7 |
| ATOM | 830 CB SER A 104 | 40 760 | 6 |
| ATOM | 831 OG SER A 104 | 12.703 31.683 47.039 1.00 28.74 | 6 |
| ATOM | 832 C SER A 104 | 32.301 31.044 45.804 1.00 35 0A | В |
| ATOM | 022 0 17 104 | 41.870 32.401 49.226 1 00 25 67 | |
| ATOM | 109 | | 6 |
| | 834 N LEU A 105 | 41 000 70 70 70 70 70 70 70 70 70 70 70 70 | 3 |
| ATOM | 835 CA LEU A 105 | 42 462 2.00 23.91 | 7 |
| ATOM | 836 CB LEU A 105 | 42 040 23.01 | 5 |
| ATOM | 837 CG LEU A 105 | 30.082 49.382 1.00 23 57 | 5 |
| MOTA | 838 CD1 LEU A 105 | 49,672 1,00 26 30 4 | |
| ATOM | 839 CD2 LEU A 105 | 39.304 30.551 49.178 1 00 22 20 | |
| | | 12 022 22 | |
| ATCM | 840 C LEU A 105 | 41 100 27.30 | • |
| MOTA | 841 O LEU A 105 | 41 604 | ; |
| ATOM | 842 N ALA A 106 | 30 31 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 | t |
| ATOM | | 33.00/ 34.556 50.897 1.00 25 32 7 | |
| ATOM | | 38.884 34.423 51.957 1 00 25 04 | |
| | | | |
| ATOM | 845 C ALA A 106 | 20 000 24.28 6 | |
| ATOM. | 846 O ALA A 106 | 20 000 | |
| ATOM | 847 N THR A 107 | 30.333 33.186 54.015 1.00 22.75 R | |
| ATOM | | 32.05/ 52.111 1 00 25 65 7 | |
| | | 39.620 30.760 52.754 1 00 25 54 | |
| MOTA | 849 CS THR A 107 | 20 700 70 70 70 70 70 70 70 70 70 70 70 7 | |
| MOTA | 850 OG1 THR A 107 | 30 550 31.713 1.00 21.92 6 | |
| ATOM | 851 CG2 THR A 107 | 30 340 30 30 30 40 8 | |
| ATOM | 852 C THR A 107 | 33.742 28.295 52.387 1.00 17.36 6 | |
| ATOM | | 30.720 53.583 1.00 20 16 6 | |
| | | 40.906 30.254 54 727 1 00 20 30 | |
| ATOM | 854 N GLY A 108 | 11 004 | |
| TCM | 855 CA GLY A 108 | 42 24 | |
| TOM · | 856 C GLY A 108 | 42 000 28.37 6 | |
| TOM | 857 O GLY A 108 | 31.921 55.019 1.00 30 26 6 | |
| TOM | | 31.499 56.076 1.00 32 op g | |
| . · · · | 858 N SER A 109 | | |
| • | | 42.283 33.018 54.942 1.00 24.81 7 | |
| | | • | |

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Figure 17-14

| ATOM | 859 | CA | SER A 109 | | 42.002 | 33.810 | 56.119 | 1.00 24.86 | c |
|---------------|------------|----------|--------------------------|---|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 860 | CE | | | 41.222 | 35.066 | 55.727 | 1.00 24.74 | 6 6 |
| ATOM | 861 | OG | SER A 109 | | 41.992 | 35.898 | 54.872 | 1.00 21.07 | 8 |
| ATOM | 862 | С | SER A 109 | | 41.240 | 32.996 | 57.173 | 1.00 27.89 | 6 |
| MOTA | 863 | 0 | SER A 109 | | 41.424 | 33.214 | 58.377 | 1.00 30.92 | 8 |
| ATOM | 864 | N | THR A 110 | | 40.389 | 32.064 | 56.744 | 1.00 23.91 | 7 |
| MOTA | 865 | CA | THR A 110 | | 39.676 | 31.259 | 57.721 | 1.00 24.80 | 6 |
| MOTA | 866 | | | • | 38.641 | 30.290 | 57.074 | 1.00 29.65 | 6 |
| ATOM | 867 | | 1 THR A 110 | | 37.469 | 31.016 | 56.669 | 1.00 30.45 | 8 |
| MOTA | 868 | | 2 THR A 110 | | 38.228 | 29.205 | 58.067 | 1.00 29.00 | 6 |
| ATOM | 869 | С | THR A 110 | - | 40.712 | 30.449 | 58.478 | 1.00 24.34 | 6 |
| ATOM | 870 | 0 | THR A 110 | | 40.615 | 30.282 | 59.699 | 1.00 24.74 | 8 |
| ATOM | 871 | | VAL A 111 | | 41.715 | 29.954 | 57.764 | 1.00 23.01 | 7 |
| MOTA | 872 | CA | | | 42.759 | 29.173 | 58.416 | 1.00 24.13 | 6 |
| ATOM | 873 874 | CB | VAL A 111 1 VAL A 111 | | 43.695 | 28.495 | 57.391 | 1.00 25.77 | 6 |
| ATOM ATOM | 875 | | 2 VAL A 111 | | 44.845 | 27.773 | 58.121 | 1.00 22.51 | 6 |
| ATOM | 876 | C C | VAL A 111 | | 42.888 43.576 | 27.502 | 56.534 | 1.00 22.67 | 6 |
| ATOM | 877 | Ö | VAL A 111 | | 43.720 | 30.071 29.793 | 59.329 | 1.00 23.14 | 6 |
| ATOM | 878 | Ŋ | GLN A 112 | • | 44.101 | 31.156 | 60.518 58.772 | 1.00 24.11 | 8 |
| ATOM | 879 | CA | GLN A 112 | | 44.895 | 32.100 | 59.554 | 1.00 24.94 1.00 25.12 | 7 6 |
| ATOM | 880 | CB | GLN A 112 | | 45.082 | 33.413 | 58.779 | 1.00 25.12 | 6 |
| ATOM | 881 | CG | GLN A 112 | | 45.545 | 33.224 | 57.330 | 1.00 28.51 | 6 |
| MOTA | 882 | CD | GLN A 112 | | 45.789 | 34.534 | 56.594 | 1.00 29.13 | 6 |
| ATOM | 883 | OE: | l GLN A 112 | | 46.779 | | 56.837 | 1.00 31.22 | 8 |
| MOTA | 884 | NE: | | | 44.877 | 34.890 | 55.694 | 1.00 29.31 | 7 |
| ATOM | 885 | c | GLN A 112 | | 44.107 | 32.362 | 60.827 | 1.00.24.62 | 6 |
| ATOM | 886 | 0 | GLN A 112 | | 44.647 | 32.311 | 61.939 | 1.00 21.10 | 8 |
| MOTA | 887 | N | ALA A 113 | | 42.813 | 32.622 | 60.644 | 1.00 24.41 | 7 |
| ATOM- ATOM | 888 889 | CA CB | ALA A 113 | | 41.914 | 32.904 | 61.751 | 1.00 23.33 | 6 |
| ATOM | 890 | C | ALA A 113 ALA A 113 | | 40.516 41.901 | 33.183 | 61.224 | 1.00 19.80 | 6 |
| ATOM | 891 | ō | ALA A 113 | | 41.925 | 31.733 31.930 | 62.729 | 1.00 25.34 | 6 |
| ATOM | 892 | N | ILE A 114 | | 41.859 | 30.509 | 63.946 62.211 | 1.00 27.52 1.00 24.39 | 8 |
| ATOM | 893 | ĊA | ILE A 114 | | 41.867 | 29.356 | 63.106 | 1.00 24.39 | 7 6 |
| ATOM | 894 | CB | ILE A 114 | | 41.524 | 28.042 | 62.371 | 1.00 23.46 | 6 |
| ATOM | 895 | CG2 | ! ILE A 114 | | 41.902 | 26.855 | 63.227 | 1.00 18.97 | 6 |
| ATOM | 896 | CG1 | ILE A 114 | | 40.030 | 28.015 | 62.034 | 1.00 21.17 | 6 |
| ATOM | 897 | | ILE A 114 | | 39.598 | 26.791 | 61.239 | 1.00 22.51 | 6 |
| ATOM | 898 | C | ILE A 114 | | 43.230 | 29.227 | 63.757 | 1.00 24.32 | 6 |
| MOTA | 899 | 0 | ILE A 114 | | 43.328 | 28.817 | 64.907 | 1.00 24.74 | 8 |
| ATOM | 900 901 | N | GLU A 1:15 | | 44.280 | 29.580 | 63.019 | 1.00 26.58 | 7 |
| MOTA MOTA | 902 | CA CB | GLU A 115 GLU A 115 | | 45.638 | 29.518 | 63.551 | 1.00 25.89 | 6 |
| ATOM | 903 | CG | GLU A 115 | | 46.639 46.554 | 29.992 29.264 | 62.508 | 1.00 22.63 | 6 |
| ATOM | 904 | CD | GLU A 115 | | 17.668 | 29.670 | 61.192 60.244 | 1.00 20.39 1.00 21.39 | 6 6 |
| ATOM | 905 | | GLU A 115 | | 47.848 | 30.887 | 60.016 | 1.00 19.60 | 8 |
| ATOM | 906 | OE2 | | | 18.362 | 28.769 | 59.722 | 1.00 22.53 | 8 |
| MOTA | 907 | С | GLU A 115 | | 45.724 | 30.422 | 64.774 | 1.00 27.56 | 6 |
| MOTA | 908 | 0 | GLU A 115 | | 46.173 | 30.006 | 65.837 | 1.00 25.98 | 8 |
| MOTA | 909 | N | GLU A 116 | | 45.267 | 31.660 | 64.615 | 1.00 31.19 | 7 |
| MOTA | 910 | CA | GLU A 116 | | 45.282 | 32.631 | 65.705 | 1.00 35.80 | 6 |
| ATOM | 911 | CB | GLU A 116 | | 44.676 | 33.959 | 65.237 | 1.00 36.91 | 6 |
| MOTA | 912 | CG | GLU A 116 | | 45.434 | 34.605 | | 1.00 41.14 | 6 |
| ATOM | 913 | CD | GLU A 116 . | | 46.872 | 34.982 | 64.420 | 1.00 43.09 | 6 |
| ATOM | 914 | | GLU A 116 | | 47.072 | 35.886 | 65.267 | 1.00 43.42 | 8 |
| ATOM | 915 916 | CE2 | GLU A 116 | | 47.802 | 34.369 | 63.849 | 1.00 41.76 | 8 |
| ATOM ATOM | 917 | 0 | GLU A 116 GLU A 116 | | 44.543 45.054 | 32.131 | 66.947 | 1.00 35.11 | 6 |
| ATOM | 918 | N | PHE A 117 | | 43.034 | 32.228 | 68.061 66.761 | 1.00 37.26 | 8 7 |
| ATOM | 919 | CA | PHE A 117 | | 42.577 | 31.598 31.096 | 67.893 | 1.00 34.30 1.00 34.44 | 5 |
| ATOM | 920 | CB | PHE A 117 | | 41.300 | 30.399 | 67.415 | 1.00 34.44 | 6 |
| ATOM | 921 | CG | PHE A 117 | | 40.383 | 29.979 | 68.533 | 1.00 33.43 | 6 |
| ATOM | 922 | | PHE A 117 | | 39.705 | 30.930 | 69.290 | 1.00 35.80 | 6 |
| ATCM | 923 | | PHE A 117 | | 40.196 | 28.630 | 68.832 | 1.00 41.05 | 6 |
| MOTA | 924 | CEl | PHE A 117 | | 38.853 | 30.549 | 70.323 | 1.00 38.08 | ·6 |

| | | • | | | | |
|--------|--------------------|--------|-----------------|----------|---|-----|
| ATOM | 925 CE2 PHE A 117 | 39.3 | | | | |
| ATOM | 926 CZ PHE A 117 | | | | | 1 6 |
| MOTA | 100 N 11/ | 38.66 | | | 7 1.00 38.64 | 6 |
| MCTA | IND A 11/ | 43.42 | | 4 68.669 | 9 1.00 34.24 | 6 |
| | 1112 X 11/ | 43.49 | 0 30.13 | 6 69.89 | B 1.00 33.54 | |
| MOTA | 929 N LEU A 118 | 44.06 | | | | 8 |
| ATOM: | - 930 CA LEU A 118 | 44.89 | | 07.53 | | 7 |
| MCTA | 931 CB LEU A 118 | | | | | : 6 |
| MOTA | 932 CG LEU A 118 | 45.15 | | | 3 1.00 30.59 | 6 |
| MOTA | 933 CD1 LEU A 118 | 43.90 | 0 25.29 | 7 67.038 | 3 1.00 27.87 | · 6 |
| | | 44.24 | 4 25.23; | 2 65.996 | 1.00 20.81 | 0 |
| ATOM | 934 CD2 LEU A 118 | 43.25 | | | | |
| MOTA | 935 C LEU A 118 | 46.21 | 6 28.696 | | | 6 |
| ATOM | 936 O LEU A 118 | 46.98 | | | | 6 |
| MOTA | 937 N LYS A 119 | | | | | 8 |
| ATOM | | 46.48 | | | 1.00 34 75 | 7 |
| | | 47.67 | 9 30.609 | 69.365 | 1.00 34.34 | |
| MOTA | 939 CB LYS A 119 | 48.14 | 3 31.739 | | | |
| MOTA | 940 CG LYS A 119 | 48.61 | | | | |
| ATOM | 941 CD LYS A 119 | 49.11. | | | | 6 |
| MOTA | 942 CE LYS A 119 | 49.69 | | | | 6 |
| ATOM | 943 NZ LYS A 119 | 43.03 | | | | 6 |
| ATOM | | 50.16 | | 64.092 | 1.00 51.48 | 7 |
| | 117 | 47.27 | 3 31.191 | 70.705 | 1.00 34.85 | |
| ATOM | 945 O LYS A 119 | 48.112 | 2 31.465 | 71.562 | | . 6 |
| ATOM | 946 N GLY A 120 | 45.967 | | | | 8 |
| MOTA | 947 CA GLY A 120 | 45.431 | | | | 7 |
| ATOM | 948 C GLY A 120 | | | | 1.00 36.25 | 6 |
| ATOM | 949 O GLY A 120 | 44.860 | | | - · · · · · · · · · · · · · · · · · · · | 6 |
| MOTA | | 44.640 | | | 1.00 46.23 | 8 |
| ATOM | | 44.619 | 33.644 | 70.586 | 1.00 38.48 | 7 |
| | 951 CA ASN A 121 | 44.079 | | 70.247 | 1.00 37.47 | |
| ATOM | 952 CB ASN A 121 | 44.928 | 35.624 | 69.170 | 1.00 37.47 | 6 |
| ATOM | 953 CG ASN A 121 | 46.340 | | | 1.00 39.57 | 6 |
| ATOM | 954 OD1 ASN A 121 | 47.078 | | 69.622 | 1.00 41.81 | 5 |
| ATOM | 955 ND2 ASN A 121 | | | 69.926 | 1.00 47.67 | 8 |
| ATOM | 956 C ASN A 121 | 46.727 | | 69.675 | 1.00 43.63 | 7 |
| ATOM | | 42.637 | 34.893 | 69.772 | 1.00 36.59 | 6 |
| | 11-20, 11 121 | 42.037 | 33.818 | 69.704 | 1.00 34.08 | |
| ATOM | 958 N VAL A 122 | 42.092 | 36.061 | 69.446 | 1.00 33.53 | 8 |
| ATOM | 959 CA VAL A 122 | 40.720 | 36.166 | 68.976 | 1.00 33.53 | 7 |
| ATOM | 960 CB VAL A 122 | 39.861 | 37.064 | | 1.00 34.77 | 6 |
| ATOM | 961 CG1 VAL A 122 | 38.418 | 37.004 | 69.898 | 1.00 38.20 | 6 |
| ATOM | 962 CG2 VAL A 122 | | 37.096 | 69.388 | 1.00 37.55 | 6 |
| ATOM | | 39.918 | 36.553 | 71.342 | 1.00 37.77 | 6. |
| ATOM | | 40.731 | 36.781 | 67.596 | 1.00 31.08 | 6 |
| | | 40.991 | 37. 9 67 | 67.441 | 1.00 34.19 | 8 |
| ATOM | 965 N ALA A 123 | 40.451 | 35.975 | 66.588 | 1.00 31.14 | 7 |
| ATOM | 966 CA ALA A 123 | 40.451 | 36.476 | 65.231 | 1.00 31.14 | |
| ATOM | 967 CB ALA A 123 | 41.307 | 35.588 | | 1.00 30.26 | 6 |
| ATOM | 968 C ALA A 123 | | | 64.327 | 1.00 32.14 | 6 |
| ATOM | 969 O ALA A 123 | 39.038 | 36.533 | 64.716 | 1.00 28.26 | 6 |
| ATOM | | 38.132 | 35.924 | 65.281 | 1.00 29.28 | 8 |
| | | 38.875 | 37.276 | 63.631 | 1.00 28.70 | 7 |
| ATOM | 971 CA PHE A 124 | 37.601 | 37.475 | 62.976 | 1.00 28.38 | |
| MCTA | 972 CB PHE A 124 | 36.920 | 38.713 | 63.563 | 1.00 20.38 | 6 |
| atom | 973 CG PHE A 124 | 35.645 | 39.099 | | 1.00 29.16 | 6 |
| ATOM | 974 CD1 PHE A 124 | | | 62.874 | 1.00 31.20 | 6 |
| MOTA | 975 CD2 PHE A 124 | 34.679 | 38.139 | | 1.00 32.00 | 6 |
| ATOM | 11 129 | 35.378 | 40.435 | 62.579 | 1.00 29.53 | 6 |
| | | 33.463 | 38.510 | 61.973 | 1.00 30.74 | 6 |
| TOM | 977 CE2 PHE A 124 | 34.165 | 40.813 | 61.988 | 1.00 27.45 | |
| -TOM | .978 CZ PHE A 124 | 33.207 | 39.847 | 61.686 | 1.00 27.45 | 6 |
| ATOM . | 979 C PHE A 124 | 37.880 | | 61.000 | 1.00 28.72 | 6 |
| NOM | 980 O PHE A 124 | | 37.671 | 61.496 | 1.00 30.19 | 6 |
| TOM | | 38.427 | 38.695 | 61.095 | 1.00 32.10 | 8 |
| | | 37.545 | 36.663 | 60.696 | 1.00 32.16 | 7 |
| TOM | 982 CA ASN A 125 | 37.731 | 36.728 | 59.251 | 1.00 30.10 | 6 |
| TOM | 983 CB ASN A 125 | 38.247 | 35.393 | 58.712 | 1 00 30.10 | |
| TOM | 984 CG ASN A 125 | 38.281 | 35.360 | 57.195 | 1.00 32.02 | 6 |
| MCT. | 985 OD1 ASN A 125 | 38.754 | | | 1.00 33.79 | 6 |
| TOM | 986 ND2 ASN A 125 | | 36.306 | 56.556 | 1.00 31.85 | 8 |
| TOM | | 37.790 | 34.268 | 56.609 | 1.00 30.51 | 7 |
| TOM | | 36.403 | 37.083 | 58.584 | 1.00 29.80 | 6 |
| TOM | 988 O ASN A 125 | 35.626 | 36.206 | 58.179 | 1.00 27.24 | 8 |
| TOM | 989 N PRO A 126 | 36.135 | 38.386 | 58.451 | 1.00 28.25 | |
| TCM | 990 CD PRO A 126 | 36.997 | 39.516 | -0.471 | 1 00 25 25 | 7 |
| .· • · | | , | JJ. J10 | 58.833 | 1.00 29.22 | 6 |

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| ATOM | 991 | CA | PRO A 126 | 34.90 | 9 38.891 | 57.844 | 1.00 27.92 | 6 |
|-------|------|-----|-----------|-------|----------|-----------------|------------|----|
| | 992 | CB | PRO A 126 | 35.13 | | 57.856 | 1.00 29.07 | 6 |
| MOTA | | | | | | | | |
| MOTA | 993 | CG | PRO A 126 | 36.64 | | 57.775 | 1.00 26.54 | 6 |
| MOTA | 994 | С | PRO A 126 | 34.65 | 1 38.339 | 56.448 | 1.00 27.54 | 6 |
| ATOM | 995 | 0 | PRO A 126 | 33.53 | 2 38.402 | 55.949 | 1.00 28.66 | 8 |
| | 996 | N | ALA A 127 | 35.68 | | 55.820 | 1.00 26.99 | 7 |
| ATOM | | | | | | | | |
| ATOM | 997 | CA | ALA A 127 | 35.54 | | 54.477 | 1.00 26.54 | 6 |
| ATOM | 998 | CB | ALA A 127 | 36.82 | 2 37.505 | 53.684 | 1.00 22.43 | 6 |
| MOTA | 999 | С | ALA A 127 | 35.22 | 5 35.744 | 54.480 | 1.00 27.38 | 6 |
| ATOM | 1000 | 0 | ALA A 127 | 35.03 | 8 35.140 | 53.423 | 1.00 29.04 | 8 |
| | 1001 | N | GLY A 128 | 35.16 | | 55.663 | 1.00 26.97 | 7 |
| MOTA | | | | | | | | |
| ATOM | 1002 | CA | GLY A 128 | 34.87 | | 55.737 | 1.00 25.65 | 6 |
| MOTA | 1003 | С | GLY A 128 | 33.38 | | 55.880 | 1.00 26.17 | 6 |
| ATOM. | 1004 | 0 | GLY A 128 | 32.60 | 0 34.428 | 55.804 | 1.00 27.39 | 8 |
| ATOM | 1005 | N | GLY A 129 | 32.99 | 8 32.234 | 56.083 | 1.00 23.87 | 7 |
| | 1006 | CA | GLY A 129 | 31.58 | | 56.236 | 1.00 25.17 | 6 |
| ATOM | | | | 30.84 | | 54.937 | 1.00 25.88 | 6 |
| MOTA | 1007 | C | GLY A 129 | | | | | |
| ATOM | 1008 | 0 | GLY A 129 | 29:64 | | 54.848 | 1.00 25.07 | 8 |
| MOTA | 1009 | N | MET A 130 | 31.56 | 6 31.198 | 53 <i>.</i> 927 | 1.00 25.69 | 7 |
| ATOM | 1010 | CA | MET A 130 | 30.98 | 1 30.872 | 52.622 | 1.00 26.48 | 6 |
| ATOM | 1011 | CB | MET A 130 | 32.10 | 3 30.907 | 51.567 | 1.00 28.53 | 6 |
| | | CG | MET A 130 | 32.79 | | 51.467 | 1.00 26.54 | 6 |
| ATOM | 1012 | | | | | 50.613 | | |
| ATOM | 1013 | SD | MET A 130 | 34.41 | | | 1.00 26.29 | 16 |
| ATOM | 1014 | CE | MET A 130 | 34.08 | | 49.062 | 1.00 25.85 | 6 |
| ATOM | 1015 | С | MET A 130 | 30.35 | 5 29.463 | 52.768 | 1.00 24.47 | 5 |
| ATOM | 1016 | 0 | MET A 130 | 30.76 | 1 28.502 | 52.113 | 1.00 17.67 | 8 |
| MOTA | 1017 | N | HIS A 131 | 29.34 | 7 29.389 | 53.636 | 1.00 23.28 | 7 |
| ATOM | 1018 | CA | HIS A 131 | 28.64 | | 54.019 | 1.00 26.33 | 6 |
| | 1019 | CB | HIS A 131 | 27.68 | | 55.180 | 1.00 26.98 | 6 |
| ATOM | | | HIS A 131 | | | | 1.00 28.50 | 6 |
| MOTA | 1020 | CG | | 26.66 | | 54.862 | | |
| ATOM | 1021 | | HIS A 131 | 26.22 | | 53.677 | 1.00 28.65 | 6 |
| MOTA | 1022 | | HIS A 131 | 25.90 | | 55.831 | 1.00 33.04 | 7 |
| ATOM | 1023 | CE1 | HIS A 131 | 25.05 | 1 30.995 | 55.259 | 1.00 27.75 | 6 |
| ATOM | 1024 | NE2 | HIS A 131 | 25.22 | 4 30.932 | 53.952 | 1.00 26.97 | 7 |
| ATOM | 1025 | C | HIS A 131 | 27.91 | 7 27.284 | 53.017 | 1.00 28.44 | 6 |
| ATOM | 1026 | ō | HIS A 131 | 27.43 | | 53.390 | 1.00 31.15 | .3 |
| | 1027 | N | HIS A 132 | 27.86 | | 51.756 | 1.00 30.64 | 7 |
| ATOM | | | | | | 50.746 | 1.00 28.71 | 6 |
| ATOM | 1028 | CA | HIS A 132 | 27.11 | | | | |
| MOTA | 1029 | CB | HIS A 132 | 26.32 | | 49.890 | 1.00 27.21 | 6 |
| ATOM | 1030 | CG | HIS A 132 | 25.40 | | 50.693 | 1.00 28.83 | 6 |
| ATOM | 1031 | CD2 | HIS A 132 | 25.11 | 1 30.137 | 50.578 | 1.00 28.92 | 6 |
| ATOM | 1032 | ND1 | HIS A 132 | 24.68 | 6 28.360 | 51.773 | 1.00 31.80 | 7 |
| ATOM | 1033 | | HIS A 132 | 23.98 | 1 29.353 | 52.285 | 1.00 29.95 | 6 |
| | 1034 | | HIS A 132 | 24.22 | | 51.579 | 1.00 28.21 | 7 |
| ATOM | | | HIS A 132 | 27.88 | | 49.851 | 1.00 28.51 | 6 |
| MOTA | 1035 | C | | | | | | 8 |
| MOTA | 1036 | 0 | HIS A 132 | 27.39 | | 49.533 | 1.00 23.44 | |
| MOTA | 1037 | N | ALA A 133 | 29.09 | | 49.455 | 1.00 27.94 | 7 |
| ATOM | 1038 | CA | ALA A 133 | 29.95 | | 48.579 | 1.00 26.99 | 6 |
| ATOM | 1039 | CB | ALA A 133 | 31.29 | 5 26.303 | 48.392 | 1.00 21.87 | 6 |
| ATOM | 1040 | С | ALA A 133 | 30.19 | 9 24.164 | 49.078 | 1.00 26.69 | 6 |
| | 1041 | ŏ | ALA A 133 | 30.70 | | 50.182 | 1.00 28.25 | 8 |
| MOTA | - | - | PHE A 134 | 29.85 | | 48.255 | 1.00 26.73 | 7 |
| ATOM | 1042 | N | | | | | | 6 |
| ATOM | 1043 | CA | PHE A 134 | 30.04 | | 48.615 | 1.00 25.04 | |
| MOTA | 1044 | CB | PHE A 134 | 29.07 | 0 20.855 | 47.875 | 1.00 19.20 | 6 |
| ATOM | 1045 | CG | PHE A 134 | 27.62 | | 48.100 | 1.00 15.75 | 6 |
| ATOM | 1046 | CD1 | | 26.92 | 9 21.960 | 47.169 | 1.00 14.83 | 6 |
| ATOM | 1047 | | PHE A 134 | 26.98 | | 49.273 | 1.00 14.03 | 6 |
| | 1048 | | PHE A 134 | 25.61 | | 47.404 | 1.00 14.84 | 6 |
| ATOM | | | | | | 49.519 | 1.00 12.07 | 6 |
| MOTA | 1049 | | PHE A 134 | 25.67 | | | | 2 |
| ATOM | 1050 | CZ | PHE A 134 | 24.98 | | 48.581 | 1.00 14.59 | 6. |
| ATOM | 1051 | С | PHE A 134 | 31.46 | | | 1.00 29.48 | 6 |
| ATOM | 1052 | 0 | PHE A 134 | 32.29 | 1 22.066 | 47.822 | 1.00 33.19 | 8 |
| ATOM | 1053 | N | LYS A 135 | 31.71 | | 48.620 | 1.00 31.52 | 7 |
| | 1054 | CA | LYS A 135 | 33.01 | | 48.427 | 1.00 29.15 | 6 |
| ATOM | | CB | LYS A 135 | 32.92 | | | 1.00 29.45 | 6 |
| ATOM | 1055 | | LYS A 135 | | | | 1.00 32.46 | 6 |
| ATOM | 1056 | CG | TID W TOO | 34.15 | 2 17.131 | ****** | | - |

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| MOTA | 105 | 7 C | D LYS A 135 | | 33.965 | 15.734 | 49,221 | 1 00 20 67 | _ |
|--------------|--------------|-----------|------------------------|---|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 105 | 8 C | | | 34.234 | | 50.716 | | 6 6 |
| ATOM | 105 | | Z LYS A 135 | | 35.679 | | 51.001 | | 7 |
| MOTA | 1060 | | LYS A 135 | | 33.513 | | 46.993 | 1.00 30.22 | 6 |
| ATOM | 106: | | LYS A 135 | | 34.714 | | 46.763 | | 8 |
| ATOM | 1062 | | | | 32.600 | | 46.028 | | 7 |
| ATOM | 1063 | | | | 32.995 | | 44.619 | | 6 |
| ATOM | 1064 | | | | 33.038 | | 44.040 | 1.00 31.41 | 6 |
| ATOM | 1065 | | | | 33.882 | | 44.810 | 1.00 35.41 | 8 |
| ATOM | 1066 1067 | | SER A 136 | | 32.097 | | 43.727 | 1.00 33.55 | 6 |
| ATOM ATOM | 1068 | | SER A 136 ARG A 137 | | 31.921 | | 42.553 | 1.00 36.11 | 8 |
| ATOM | 1069 | | | | 31.536 | | 44.262 | 1.00 30.61 | 7 |
| ATOM | | | | | 30.664 29.324 | | 43.459 | 1.00 32.28 | 6 |
| ATOM | 1071 | | | | 28.224 | 21.554 22.458 | 43.202 42.627 | 1.00 35.91 | 6 |
| ATOM | 1072 | | | | 26.819 | 21.836 | 42.027 | 1.00 43.90 | 6 |
| ATOM | 1073 | | | • | 26.571 | 20.767 | 41.787 | 1.00 48.28 1.00 53.38 | 6 |
| ATOM | 1074 | CZ | | | 26.150 | | 40.538 | 1.00 55.30 | 7 5 |
| MOTA | 1075 | NH | 11 ARG A 137 | | 25.921 | 22.185 | 40.090 | 1.00 54.06 | 7 |
| MOTA | 1076 | NH | 12 ARG A 137 | | 25.969 | 19.922 | 39.728 | 1.00 58.96 | 7 |
| MOTA | 1077 | | ARG A 137 | | 30.405 | 23.631 | 44.113 | 1.00 30.24 | 6 |
| ATOM | 1078 | | ARG A 137 | | 30.380 | 23.748 | 45.338 | 1.00 23.11 | 8 |
| MOTA | 1079 | | ALA A 138 | | 30.219 | 24.653 | 43.279. | 1.00 27.33 | 7 |
| ATOM | 1080 1081 | | | | 29.944 | 26.000 | 43.757 | 1.00 27.36 | 6 |
| MOTA MOTA | 1081 | | ALA A 138 ALA A 138 | | 30.149 | 26.997 | 42.645 | 1.00 27.57 | 6 |
| MOTA | 1083 | | ALA A 138 | | 28.496 | 26.003 | 44.213 | 1.00 26.45 | 6 |
| ATOM | 1084 | N | ASN A 139 | | 27.747 28.090 | 25.083 27.021 | 43.865 | 1.00 27.30 | 8 |
| ATOM | 1085 | CA | | | 26.711 | 27.021 | 44.975 45.471 | 1.00 22.47 | 7 |
| ATOM | 1086 | CB | ASN A 139 | | 26.406 | 25.738 | 46.218 | 1.00 23.85 1.00 16.82 | 6 |
| MOTA | 1087 | CG | ASN A 139 | | 25.040 | 25.718 | 46.900 | 1.00 14.45 | 6 6 |
| ATOM | 1088 | OD. | 1 ASN A 139 | | 24.019 | 26.084 | 46.319 | 1.00 13.39 | 8 |
| ATOM | 1089 | ND: | | | 25.018 | 25.249 | 48.139 | 1.00 20.08 | 7 |
| MOTA | 1090 | С | ASN A 139 | | 26.444 | 28.277 | 46.368 | 1.00 26.09 | 6 |
| ATOM | 1091 | 0 | ASN A 139 | | 27.239 | 28.600 | 47.260 | 1.00 27.50 | 8 |
| ATOM ATOM | 1092 1093 | N CA | GLY A 140 | | 25.326 | 28.954 | 46.114 | 1.00 24.83 | 7 |
| ATOM | 1094 | CA | GLY A 140 GLY A 140 | | 24.965 | 30.106 | 46.916 | 1.00 22.24 | 6 |
| ATOM | 1095 | õ | GLY A 140 | | 25.991 26.256 | 31.211 31.843 | 46.890 | 1.00 22.35 | 6 |
| ATOM | 1096 | N | PHE A 141 | | 26.570 | 31.437 | 47.910 45.717 | 1.00 23.50 | 8 |
| ATOM | 1097 | CA | PHE A 141 | | 27.582 | 32.476 | 45.518 | 1.00 25.60 1.00 26.47 | 7 6 |
| MOTA | 1098 | CB | PHE A 141 | | 27.204 | 33.765 | 46.258 | 1.00 28.05 | 6 |
| ATOM | 1099 | CG | PHE A 141 | | 25.925 | 34.391 | 45.792 | 1.00 28.61 | 6 |
| ATOM | 1100 | | PHE A 141 | | 25.352 | 35.428 | 46.518 | 1.00 30.74 | 6 |
| ATOM | 1101 | CD2 | | | 25.312 | 33.975 | 44.620 | 1.00 29.10 | 6 |
| MO A | 1102 | CEI | | | 24.193 | 36.044 | 46.087 | 1.00 29.33 | 6 |
| ATOM ATOM | 1103 1104 | CE2 | PHE A 141 PHE A 141 | - | 24.150 | 34.583 | 44.177 | 1.00 31.03 | 6 |
| ATOM | 1105 | -0 | PHE A 141 | | 23.589 | 35.621 | 44.912 | 1.00 32.59 | 6 |
| MOTA | 1106 | o | PHE A 141 | | 28.954 29.938 | 32.038 32.727 | 45.991 45.733 | 1.00 24.63 | 6 |
| ATOM | 1107 | N | CYS A 142 | | 29.025 | | 46.667 | 1.00 29.72 | 8 |
| MOTA | 1108 | CA | CYS A 142 | | 30.296 | 30.399 | 47.192 | 1.00 21.11 1.00 22.30 | 7 |
| MOTA | 1109 | CB | CYS A 142 | | 30.062 | 29.787 | 48.567 | 1.00 21.31 | 6 6 |
| MOTA | 1110 | SG | CYS A 142 | | 28.943 | 30.748 | 49.582 | 1.00 22.93 | 16 |
| MOTA | 1111 | С | CYS A 142 | | 31.017 | 29.366 | 46.326 | 1.00 22.13 | 6 |
| ATOM | 1112 | 0 | CYS A 142 | | 30.408 | 28.389 | 45.878 | 1.00 22.97 | 8 |
| ATOM | 1113 | N | TYR A 143 | | 32.317 | 29.573 | 46.111 | 1.00 23.09 | 7 |
| ATOM | 1114 | CA | TYR A 143 | | 33.129 | 28.632 | 45.335 | 1.00 23.05 | 6 |
| MOTA | 1115 | CB | TYR A 143 | | 34.063 | 29.365 | 44.375 | 1.00 21.60 | 6 |
| ATOM | 1116 | CG CD1 | TYR A 143 | | 33.377 | 30.379 | 43.487 | 1.00 24.09 | 6 |
| ATOM | 1117 1118 | | TYR A 143 TYR A 143 | | 32.969 | 31.609 | 43.999 | 1.00 23.29 | 6 |
| ATOM ATOM | 1119 | | TYR A 143 | | 32.365 33.154 | 32.555 | 43.199 | 1.00 23.26 | 6. |
| ATOM | 1120 | | TYR A 143 | | 32.544 | 30.117 31.061 | 42.135 | 1.00 22.52 | 6 |
| ATOM | 1121 | CZ | TYR A 143 | | 32.153 | 32.281 | 41.317 41.857 | 1.00 24.82 1.00 27.55 | 6 6 |
| ATOM | 1122 | OH | TYR A 143 | | 31.553 | 33.241 | 41.064 | 1.00 32.35 | 8 |
| · · · · · · | | | | | | 241 | | 2.00 34.33 | J |

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i

| MOTA | 1123 | С | TYR A | 143 | | 33.960 | 27.766 | 46.290 | 1.00 24.22 | 6 |
|--------------|------|-----|--------|-----|---|--------|---------|--------|-------------|-----|
| | 1124 | ō | TYR A | | | 34.266 | 26.606 | 45.998 | 1.00 24.58 | 8 |
| ATOM | 1125 | N | ILE A | | | 34.327 | 28.329 | 47.437 | 1.00 23.83 | 7 |
| MOTA | 1126 | CA | ILE A | | | 35.086 | 27.566 | 48.425 | 1.00 20.24 | 6 |
| ATOM | 1127 | CB | ILE A | | | 36.547 | 27.982 | 48.453 | 1.00 17.27 | 6 |
| MOTA | | | ILE A | | | 37.231 | 27.354 | 49.662 | 1.00 11.03 | 6 |
| ATOM | 1128 | | | | | 37.185 | 27.603 | 47.110 | 1.00 14.93 | 6 |
| MOTA | 1129 | _ | ILE A | | | 38.601 | 28.028 | 46.946 | 1.00 19.68 | 6 |
| ATOM | 1130 | | ILE A | | | | 27.703 | 49.815 | 1.00 21.77 | 6 |
| MOTA | 1131 | C | ILE A | | | 34.495 | | 50.318 | 1.00 21.77 | 8 |
| ATOM | 1132 | 0 | ILE A | | | 34.288 | 28.811 | | | 7 |
| MOTA | 1133 | N | ASN A | | • | 34.212 | 26.555 | 50.424 | 1.00 23.00 | 6 |
| ATOM | 1134 | CA | ASN A | | | 33.616 | 26.508 | 51.750 | 1.00 20.92 | |
| ATOM | 1135 | CB | asn a | | | 32.902 | 25.170 | 51.935 | 1.00 17.08 | 6 |
| MOTA | 1136 | CG | ASN A | | | 32.079 | 25.125 | 53.203 | 1.00 21.04 | 6 |
| MOTA | 1137 | | ASN A | | | 32.549 | 25.508 | 54.276 | 1.00 20.97 | 8 |
| MOTA | 1138 | ND2 | asn a | 145 | | 30.844 | 24.640 | 53.093 | 1.00 20.93 | 7 |
| MOTA | 1139 | С | ASN A | 145 | | 34.706 | 26.669 | 52.806 | 1.00 19.68 | 6 |
| ATOM | 1140 | 0 | ASN A | 145 | | 35.201 | 25.679 | 53.351 | 1.00 20.64 | . 8 |
| MOTA | 1141 | N | ASN A | 146 | | 35.079 | 27.911 | 53.100 | 1.00 16.28 | 7 |
| ATOM | 1142 | CA | ASN A | 146 | | 36.123 | 28.143 | 54.088 | 1.00 19.34 | 6 |
| ATOM | 1143 | CB | ASN A | 146 | | 36.428 | 29.651 | 54.207 | 1.00 20.27 | 6 |
| ATOM | 1144 | CG | ASN A | 146 | | 35.292 | 30.444 | 54.795 | 1.00 18.05 | 6 |
| ATOM | 1145 | OD1 | ASN A | 146 | | 35.079 | 30.421 | 55.999 | 1.00 25.83 | 8 |
| ATOM | 1146 | ND2 | ASN A | 146 | | 34.552 | 31.149 | 53.948 | 1.00 16.04 | 7 |
| MOTA | 1147 | С | ASN A | 146 | | 35.775 | 27.504 | 55.443 | 1.00 20.48 | 6 |
| ATOM | 1148 | 0 | ASN A | 146 | | 36.663 | 27.027 | 56.151 | 1.00 19.88 | 8 |
| ATOM | 1149 | N | PRO A | | | 34.482 | 27.485 | 55.819 | 1.00 19.38 | 7 |
| ATOM | 1150 | CD | PRO A | | | 33.312 | 28.068 | 55.135 | 1.00 17.48 | 6 |
| ATOM | 1151 | CA | PRO A | | | 34.058 | 26.877 | 57.087 | 1.00 22.25 | 6 |
| ATOM | 1152 | CB | PRO A | | | 32.539 | 27.065 | 57.057 | 1.00 20.15 | 6 |
| ATOM | 1153 | CG | PRO -A | | | 32.407 | 28.378 | 56.305 | 1.00 20.81 | 6 |
| ATOM | 1154 | C | PRO A | | | 34.443 | 25.383 | 57.188 | 1.00 26.89 | 6 |
| ATOM | 1155 | 0 | PRO A | | | 35.066 | 24.954. | 58.169 | 1.00 29.10 | 8 |
| ATOM | 1156 | N | ALA A | | | 34.070 | 24.596 | 56.176 | 1.00 25.88 | 7 |
| ATOM | 1157 | CA | ALA A | | | 34.372 | 23.164 | 56.174 | 1.00 25.47 | 6 |
| ATOM | 1158 | CB | ALA A | | | 33.670 | 22.468 | 55.009 | 1.00 21.84 | 6 |
| ATOM | 1159 | c | ALA A | | | 35.870 | 22.916 | 56.100 | 1.00 25.94 | 6 |
| ATOM | 1160 | Õ | ALA A | | | 36.382 | 21.971 | 56.701 | 1.00 27.19 | 8 |
| ATOM | 1161 | N | VAL A | | | 36.574 | 23.756 | 55.349 | 1.00 26.11 | 7 |
| ATOM | 1162 | CA | VAL A | | | 38.017 | 23.609 | 55.233 | 1.00 24.04 | ` 6 |
| ATOM | 1163 | CB | VAL A | | | 38.622 | 24.663 | 54.267 | 1.00 26.16 | 6 |
| MOTA | 1164 | | VAL A | | | 40.135 | 24.476 | 54.158 | 1.00 25.36 | 6 |
| ATOM | 1165 | | VAL A | | | 37.970 | 24.544 | 52.886 | 1.00 26.81 | 6 |
| ATOM | 1166 | С | VAL A | | | 38.516 | 23.870 | 56.640 | 1.00 23.57 | 6 |
| ATOM | 1167 | Ō | VAL A | | | 39.453 | 23.228 | 57.122 | 1.00 19.75 | 8 |
| ATOM | 1168 | N | GLY A | | | 37.850 | 24.815 | 57.299 | 1.00 22.20 | 7 |
| ATOM | 1169 | CA | GLY A | | | 38.210 | 25.175 | 58.654 | 1.00 25.43 | 6 |
| | 1170 | C | GLY A | | | 38.130 | 23.975 | 59.568 | 1.00 27.19 | 6 |
| MOTA MOTA | 1171 | ō | GLY A | | | 39.112 | 23.620 | 60.221 | 1.00 27.05 | 8 |
| ATOM | 1172 | N | ILE A | | | 36.959 | 23.348 | 59.618 | 1.00 25.56 | 7 |
| ATOM | 1173 | CA | ILE A | | | 36.775 | 22.176 | 60.457 | 1.00 28.24 | 6 |
| | 1174 | CB | ILE A | | | 35.317 | 21.654 | 60.389 | .1.00 29.41 | 6 |
| ATOM ATOM | 1175 | | ILE A | | | 35.251 | 20.215 | 60.869 | 1.00 26.02 | 6 |
| | 1176 | | ILE A | | | 34.394 | 22.540 | 61.240 | 1.00 33.31 | 6 |
| MOTA | 1177 | | ILE A | | | 34.255 | 23.967 | 60.759 | 1.00 36.83 | 6 |
| MOTA | 1178 | C | ILE A | | | 37.723 | 21.039 | 60.075 | 1.00 29.32 | 6 |
| MOTA | 1179 | ŏ | ILE A | | | 38.340 | 20.420 | 60.947 | 1.00 29.08 | 8 |
| MOTA | 1180 | N | GLU A | 152 | | 37.843 | 20.769 | 58.778 | 1.00 29.91 | 7 |
| MOTA | 1181 | CA | GLU A | | | 38.704 | 19.690 | 58.315 | 1.00 32.58 | 6 |
| ATOM | 1182 | CB | GLU A | | | 38.575 | 19.526 | 56.802 | 1.00 35.07 | 6 |
| ATCM | 1182 | CG | GLU A | | | 37.269 | 13.848 | 56.393 | 1.00 38.51 | 6 |
| ATOM | | CD | GLU A | | | 37.120 | 17.440 | 56.987 | 1.00 41.41 | 6 |
| ATOM | 1184 | OE1 | | 152 | | 36.089 | 16.779 | 56.718 | 1.00 45.64 | 8 |
| atom | 1185 | OE2 | | | | 38.030 | 16.992 | 57.723 | 1.00 40.09 | 8 |
| ATOM | 1186 | C | GLU A | | | 40.145 | 19.903 | 58.721 | 1.00 32.97 | 6 |
| ATOM | 1187 | 0 | GLU A | | | 40.879 | 18.946 | 58.978 | 1.00 30.15 | 8 |
| ATOM | 1188 | υ. | GDO W | | | 40.07 | 10.550 | - | | |
| • • | | | CHID | · | | | | | | |

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Figure 17-19

| ATOM | 1189 | N TYR A 153 | 40.54 | 1 21.170 | 58.765 | 1.00 33.90 | - |
|--------------|--------------------|--------------------------------|------------------|------------------|------------------|--------------------------|--------|
| MOTA | | CA TYR A 153 | 41.87 | | | 1.00 33.90 | 7 6 |
| MOTA | | B TYR A 153 | 42.01 | 9 23.074 | 59.058 | | 6 |
| MOTA | | CG TYR A 153 | 43.28 | | 59.639 | 1.00 38.03 | 6 |
| ATOM ATOM | | CD1 TYR A 153 CE1 TYR A 153 | 44.49 | | 58.948 | 1.00 42.34 | 6 |
| MOTA | | D2 TYR A 153 | 45.65 | _ | | | 6 |
| MCTA | | E2 TYR A 153 | 43.25 44.38 | _ | | | 6 |
| ATOM | | Z TYR A 153 | 45.58 | | | | 6 |
| ATOM | | H .TYR A 153 | 46.69 | | | | 6 |
| ATOM | 1199 C | TYR A 153 | 41.919 | | 60.667 | 1.00 44.86 1.00 32.59 | 8 |
| atom | 1200 C | | 42.86 | | | 1.00 32.39 | 6 8 |
| ATOM. | 1201 N | | 40.869 | 21.556 | 61.397 | | 7 |
| MOTA | | A LEU A 154 | 40.730 | | 62.823 | 1.00 29.38 | 6 |
| ATOM ATOM | | B LEU A 154 G LEU A 154 | 39.443 | | | 1.00 28.60 | 6 |
| ATOM | | D1 LEU A 154 | 39.399 | | | | 6. |
| ATOM | 1206 C | D2 LEU A 154 | 37.991 40.418 | | 64.041 | | 6 |
| ATOM | 1207 C | | 40.732 | | 64.691 63.146 | 1.00 24.95 | 6 |
| MCTA | 1208 O | | 41.223 | | | 1.00 29.56 1.00 28.36 | 6 |
| ATOM | 1209 N | | 40.174 | | 62.256 | 1.00 20.36 | 8 7 |
| ATOM | 1210 C | | 40.134 | 17.522 | 62.499 | 1.00 33.00 | 6 |
| ATOM | 1211 C | | 39.127 | | 61.561 | 1.00 33.13 | 6 |
| MOTA MOTA | 1212 C | | 37.708 | | 61.769 | 1.00 32.84 | 6 |
| ATOM | 1213 CI 1214 NI | | 36.678 | | 60.863 | 1.00 32.92 | 6 |
| ATOM | 1215 C | | 36.152 35.195 | | 61.363 | 1.00 33.98 | 7 |
| ATOM | | 11 ARG A 155 | 34.671 | | 60.741 | 1.00 37.93 | 6 |
| ATOM | | 12 ARG A 155 | 34.732 | | 59.605 61.259 | 1.00 38.39 | 7 |
| ATOM | 1218 C | ARG A 155 | 41.521 | 16.929 | 62.331 | 1.00 38.67 1.00 33.97 | 7 |
| ATOM | 1219 0 | ARG A 155 | 41.869 | 15.941 | 62.985 | 1.00 33.97 | 6 8 |
| MOTA | 1220 N | LYS A 156 | 42.318 | 17.548 | 61.467 | 1.00 34.20 | 7 |
| ATOM | 1221 CA | | 43.679 | 17.081 | 61.243 | 1.00 36.32 | 6 |
| ATOM ATOM | 1222 CE 1223 CG | | 44.249 | 17.662 | 59.942 | 1.00 37.57 | 6 |
| ATOM | 1224 CE | | 45.673 46.116 | 17.187 | 59.638 | 1.00 40.32 | 6 |
| ATOM | 1225 CE | | 45.180 | 17.532 16.909 | 58.220 57.184 | 1.00 40.33 | 6 |
| ATOM | 1226 NZ | | 45.015 | 15.435 | 57.364 | 1.00 41.27 1.00 37.92 | 6 |
| MCTA | 1227 C | LYS A 156 | 44.539 | 17.501 | 62.428 | 1.00 37.92 | 7 6 |
| MOTA | 1228 0 | LYS A 156 | 45.582 | 16.905 | 62.699 | 1.00 34.53 | . 8 |
| MCTA | 1229 N | LYS A 157 | 44.093 | 18.537 | 63.132 | 1.00 36.71 | 7 |
| MOTA MOTA | 1230 CA 1231 CB | | 44.820 | 19.026 | 64.294 | 1.00 37.09 | 6 |
| MOTA | 1232 CG | | 44.495 | 20.501 | 64.566 | 1.00 37.02 | 6 |
| ATOM | 1233 CD | LYS A 157 | 44.982 46.468 | 21.435 21.231 | 63.477 | 1.00 36.22 | 6 |
| MCTA | 1234 TE | LYS A 157 | 46.993 | 22.100 | 63.239 62.107 | 1.00 37.91 | 6 |
| MOTA | 1235 JZ | LYS À 157 | 48.434 | 21.815 | 61.842 | 1.00 39.35 1.00 38.78 | 6 7 |
| MCTA | 1236 | LYS A 157 | 44.498 | 18.178 | 65.515 | 1.00 35.61 | 6 |
| ATOM | 1237 0 | LYS A 157 | 45.204 | 18.232 | 66.518 | 1.00 36.38 | 8 |
| MOTA | 1238 N | GLY A 158 | 43.433 | 17.392 | 65.431 | 1.00 34.37 | 7 |
| MOTA MOTA | 1239 CA 1240 C | GLY A 158 | 43.097 | 16.537 | 66.552 | 1.00 38.08 | 6 |
| ATCM | 1241 0 | GLY A 158 GLY A 158 | 41.782 | 16.781 | 67.267 | 1.00 38.78 | 6 |
| ATOM | 1242 N | PHE A 159 | 41.460 41.023 | 16.053 17.791 | 68.208 | 1.00 41.07 | 8 |
| MOTA | 1243 CA | PHE A 159 | 39.743 | 18.046 | 66.855 67.505 | 1.00 36.75 | 7 |
| ATOM | 1244 CB | PHE A 159 | 39.246 | 19.459 | 67.213 | 1.00 33.83 | 6 |
| MCTA | 1245 CG | PHE A 159 | 40.115 | 20.521 | 67.787 | 1.00 32.65 1.00 29.97 | 6 6 |
| MCTA | 1246 CD1 | PHE A 159 | 41.404 | 20.724 | 67.297 | 1.00 30.20 | 6 |
| MOTA | 1247 CD2 | PHE A 159 | 39.672 | 21.289 | 68.853 | 1.00 29.28 | 6 |
| MOTA | 1248 CE1 | PHE A 159 | 42.241 | 21.680 | 67.862 | 1.00 28.96 | 6 |
| ATOM | | PHE A 159 | 40.498 | 22.246 | 69.428 | 1.00 29.67 | 6 |
| MCTA MCTA | 1250 CZ 1251 C | PHE A 159 PHE A 159 | 41.785 | 22.442 | 68.931 | 1.00 30.59 | 6 |
| ATCM | 1252 0 | PHE A 159 | 38.732 38.664 | 17.026 16.716 | 67.025 | 1.00 33.41 | 6 |
| ATCM | 1253 N | LYS A 160 | 37.951 | 16.716 | 65.838 | 1.00 31.61 | 8 |
| MOTA | 1254 CA | LYS A 160 | 36.947 | 15.493 | 67.966 67.677 | 1.00 35.13 1.00 35.39 | 7 |
| | ٠. | | | 40.400 | 9/.0// | 1.00 35.39 | 6 |

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| | 1055 | | | | | | | |
|--------|-----------|---------------|---|--------|--------|---------------------|------------|-----|
| ATOM | | CB LYS A 160 | | 37.342 | 14.198 | 68.389 | 1.00 36.43 | 6 |
| ATOM | 1256 | CG LYS A 160 | | 38.535 | 13.502 | 67.708 | 1.00 40.67 | |
| | | | | | | | 1.00 40.67 | - 6 |
| ATOM | | CD LYS A 160 | | 39.312 | 12.538 | 68.615 | 1.00 44.68 | 6 |
| ATOM | 1258 | CE LYS A 160 | | 38.425 | 11.536 | 69.345 | 1.00 49.23 | |
| | | | | | | | | 6 |
| ATOM | | | | 37.593 | 12.182 | 70.411 | 1.00 50.63 | 7 |
| MOTA | 1260 | C LYS A 160 | | 35.524 | 15.927 | 68.027 | 1.00 35.94 | |
| MOTA | 1261 | O LYS A 160 | | | | | | 6 |
| | | | | 34.561 | 15.241 | 67.691 | 1.00 35.72 | 8 |
| ATOM | 1262 | N ARG A 161 | • | 35.399 | 17.058 | 68.718 | 1.00 34.35 | 7 |
| MOTA | 1263 | CA ARG A 161 | | | | | 2.00 34.33 | |
| | | | | 34.091 | 17.618 | 69.044 | 1.00 34.95 | 6 |
| ATOM | 1264 | C9 ARG A 161 | | 33.771 | 17.525 | 70.535 | 1.00 33.94 | 6 |
| ATOM | 1265 | CG ARG A 161 | | 33.427 | 16.132 | 70.992 | | |
| | | | • | | | | 1.00 38.25 | 6 |
| MOTA | | CD ARG A 161 | | 32.823 | 16.131 | 72.386 | 1.00 41.17 | 6 |
| ATOM | 1267 | NE ARG A 161 | | 33.719 | 16,722 | 73.378 | 1.00 47.64 | |
| ATOM | 1268 | CZ ARG A 161 | | | | | | 7 |
| | | 20 ANG A 101 | | 34.912 | 16.233 | 73.705 | 1.00 47.92 | 6 |
| ATOM | 1269 I | NH1 ARG A 161 | | 35.372 | 15.131 | 73.121 | 1.00 47.56 | 7 |
| MOTA | 1270 I | VH2 ARG A 161 | | 35.648 | 16.858 | 74.516 | | |
| | | | | | | | 1.00 46.95 | 7 |
| ATOM | 1271 (| | | 34.113 | 19.076 | 68.5 9 8 | 1.00 34.58 | 6 |
| MOTA | 1272 (| D ARG A 161 | | 34.468 | 19.980 | 69.357 | 1.00 33.77 | |
| ATOM | | ILE A 162 | | | | | 1.00 33.77 | 8 |
| | | | | 33.741 | 19.280 | 67.341 | 1.00 31.74 | 7 |
| MOTA | 1274 | CA ILE A 162 | | 33.735 | 20.594 | 66.735 | 1.00 29.83 | . 6 |
| ATOM | 1275 C | B ILE A 162 | | 34.429 | 20.542 | | 1 00 25.05 | |
| | | | | | | 65.362 | 1.00 29.96 | 6 |
| ATOM | 1276 C | G2 ILE A 162 | | 34.580 | 21.942 | 64.784 | 1.00 30.57 | 6 |
| ATOM | 1277 C | G1 ILE A 162 | | 35.801 | 19.891 | 65.522 | 1.00 28.81 | |
| ATOM | 1278 0 | D1 ILE A 162 | | | | | | 6 |
| | | | | 36.537 | 19.685 | 64.224 | 1.00 33.05 | 6 |
| ATOM | 1279 C | ILE A 162 | | 32.300 | 21.050 | 66.560 | 1.00 29.66 | 6 |
| ATOM | 1280 C | ILE A 162 | | 31.416 | 20.241 | 66.266 | 1.00 25.24 | |
| ATOM | 1281 N | | | | | | 1.00 25.24 | 8 |
| | | DEU A 103 | | 32.081 | 22.351 | 66.745 | 1.00 30.00 | 7 |
| MOTA | 1282 C | A LEU A 163 | | 30.754 | 22.945 | 66.617 | 1.00 30.48 | 6 |
| ATOM | 1283 C | B LEU A 163 | | 30.236 | 23.406 | 67.992 | 1.00 32.25 | |
| MOTA | | G LEU A 163 | | | | | 1.00 32.23 | 6 |
| | | | | 28.934 | 24.229 | 68.044 | 1.00 31.21 | 6 |
| ATOM | 1285 C | D1 LEU A 163 | | 27.804 | 23.494 | 67.326 | 1.00 31.58 | 6 |
| ATOM | 1286 C | D2 LEU A 163 | | 28.569 | 24.502 | 69.493 | 1.00 25.00 | |
| ATOM | 1287 C | | | | | | 1.00 25.00 | Ġ |
| | _ | | | 30.717 | 24.122 | 65.659 | 1.00 29.23 | 6 |
| MOTA | 1288 0 | LEU A 163 | | 31.596 | 24.980 | 65.654 | 1.00 29.72 | 8 |
| ATOM | 1289 N | TYR A 164 | | 29.675 | 24.157 | 64.846 | | |
| | 1290 C | | | | | | 1.00 29.68 | 7 |
| ATOM | | | | 29.500 | 25.244 | 63.899 | 1.00 29.89 | 6 |
| ATOM | 1291 C | B TYR A 164 | | 29.512 | 24.688 | 62.470 | 1.00 27.81 | 6 |
| ATOM | 1292 C | G TYR A 164 | | 29.377 | 25.742 | 61.399 | 1.00 27.79 | |
| ATOM | | D1 TYR A 164 | | | | | | 6 |
| | | | | 30.390 | 26.670 | 61.168 | 1.00 24.82 | 6 |
| MOTA | _1294 C | E1 TYR A 164 | | 30.247 | 27.655 | 60.198 | 1.00 24.51 | 6 |
| MOTA | 1295 CI | D2 TYR A 164 | | 28.216 | 25.827 | 60.631 | 1.00 27.61 | 6 |
| ATOM | | E2 TYR A 164 | | | | | | |
| | | | | 28.065 | 26.808 | 59.662 | 1.00 25.67 | 5 |
| ATOM | 1297 C | Z TYR A 164 | | 29.078 | 27.718 | 59.451 | 1.00 25.63 | 6 |
| ATOM | 1298 OF | TYR A 164 | | 28.898 | 28.704 | 58.506 | | |
| | 1299 C | | | | | | 1.00 27.10 | 8 |
| ATOM | | TYR A 164 | | 28.149 | 25.907 | 64.218 | 1.00 28.38 | 6 |
| ATOM | 1300 O | TYR A 164 | | 27.119 | 25.225 | 64.277 | 1.00 29.43 | 8 |
| ATOM | 1301 N | ILE A 165 | | 28.166 | 27.217 | 64.464 | | |
| | | | | | | | 1.00 24.30 | 7 |
| ATOM | _ | | | 26.941 | 27.969 | -64.754 | 1.00 22.93 | 6 |
| MOTA | 1303 CE | 3 ILE A 165 | | 26.985 | 28.649 | 66.143 | 1.00 22.00 | 6 |
| ATOM | 1304 CG | | | 25.765 | | | | |
| | | | | | 29.559 | 66.312 | 1.00 16.15 | 6 |
| MOTA | 1305 CG | | | 27.033 | 27.567 | 67.240 | 1.00 20.78 | 6 |
| ATOM | 1306 CE | 1 ILE A. 165 | | 27.185 | 28.101 | 68.650 | 1.00 15,49 | 6 |
| ATOM | 1307 C | ILE A 165 | | 26.784 | | | | |
| | | THE A 105 | | | 29.010 | 63.657 | 1.00 24.45 | 6 |
| MOTA | 1308 ఫ | ILE A 165 | | 27.605 | 29.921 | 63.506 | 1.00 23.17 | 8 |
| ATOM | 1309 N | ASP A 166 | | 25.709 | 28.871 | 62.895 | 1.00 24.20 | 7 |
| | 1310 CA | | | | | | | |
| MOTA | | WOL W TOO | | 25.478 | 29.726 | 61.749 | 1.00 20.78 | 6 |
| ATOM | 1311 CB | | | 25.314 | 28.809 | 60.548 | 1.00 17.64 | 6 |
| ATOM | 1312 CG | ASP A 166 | | 25.410 | 29.529 | 59.256 | 1.00 19.93 | 6 |
| ATOM | | 1 ASP A 166 | | | | | | |
| | 1313 00 | | | 24.536 | 30.391 | 59.004 | 1.00 20.20 | 8 |
| MOTA | | 2 ASP A 166 | | 26.366 | 29.231 | 58.491 | 1.00 17.64 | 8 |
| ATOM | 1315 C | ASP A 166 | | 24.290 | 30.670 | 61.895 | 1.00 22.79 | 6 |
| | 1316 0 | | | | | | | |
| ATOM | | ASP A 166 | | 23.134 | 30.256 | 61.826 | 1.00 22.70 | . 8 |
| ATOM | 1317 N | LEU A 167 | | 24.583 | 31.952 | 62.085 | 1.00 25.40 | 7 |
| ATOM . | 1318 CA | LEU A 167 | | 23.536 | 32.954 | 62.250 | 1.00 25.76 | 6 |
| | 1319 CB | LEU A 167 | | | | | 1 00 25 75 | |
| MOTA | | | | 23.963 | 33.991 | 63.288 | 1.00 26.65 | 6 |
| MOTA | 1320, "ÇG | LEU A 167 | | 24.364 | 33.463 | 64.674 | 1.00 26.75 | 6 |

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| ATOM | 1321 | CD | 1 LEU A 167 | | 24.741 | 34.647 | 65.552 | 1.00 26.24 | 6 |
|--------|------|-----|--------------|---|--------|--------|-----------------|------------|-----|
| ATOM | 1322 | | 2 LEU A 167 | | 23.225 | 32.661 | 65.302 | 1.00 23.45 | |
| MOTA | 1323 | c | LEU A 167 | | 23.162 | | | | 6 |
| | | | | | | 33.660 | 60.951 | 1.00 26.37 | 6 |
| ATOM | 1324 | 0 | LEU A 167 | | 22.386 | 34.613 | 60.971 | 1.00 25.95 | 8 |
| ATOM | 1325 | N | ASP A 168 | | 23.726 | 33.208 | 59.828 | 1.00 29.66 | 7. |
| ATOM- | 1326 | CA | ASP A 168 | | 23.410 | 33.787 | 58.520 | 1.00 28.35 | 6 |
| ATOM | 1327 | CB | ASP A 168 | | 24.057 | 32.987 | 57.390 | 1.00 33,29 | 6 |
| ATOM | 1328 | CG | | | 23.937 | 33.676 | 56.037 | 1.00 35.38 | |
| ATOM | 1329 | | 1 ASP A ·168 | | 24.892 | | | | 6 |
| | | | | | | 34.388 | 55.659 | 1.00 39.48 | 8 |
| MOTA | 1330 | | 2 -ASP A 168 | | 22.893 | 33.531 | 55.364 | 1.00 33.40 | 8 |
| ATOM | 1331 | С | ASP A 168 | | 21.906 | 33.614 | 58.408 | 1.00 28.74 | 6 |
| ATOM | 1332 | 0 | ASP A 168 | | 21.354 | 32.648 | 58.948 | 1.00 26.21 | 8 |
| ATOM | 1333 | N | ALA A 169 | - | 21.239 | 34.524 | 57.711- | 1.00 26.16 | 7 |
| ATOM | 1334 | CA | ALA A 169 | | 19.793 | 34.415 | 57.579 | 1.00 24.39 | 6 |
| ATOM | 1335 | CB | ALA A 169 | | 19.233 | 35.640 | 56.879 | 1.00 22.75 | |
| | 1336 | | | | | | | | 6 |
| MOTA | | C | ALA A 169 | | 19.420 | 33.157 | 56.813 | 1.00 24.37 | 6 - |
| ATOM | 1337 | 0 | ALA A 169 | | 18.266 | 32.752 | 56.824 | 1.00 22.34 | 8 |
| MOTA | 1338 | N | HIS A 170 | | 20.405 | 32.542 | 56.156 | 1.00 25.78 | 7 |
| ATOM | 1339 | CA | HIS A 170 | | 20.180 | 31.327 | 55.375 | 1.00 25.20 | 6 |
| ATOM | 1340 | CB | HIS A 170 | | 20.667 | 31.501 | 53.936 | 1.00 25.76 | 6 |
| ATOM | 1341 | CG | HIS A 170 | | 20.122 | 32.711 | 53.245 | 1.00 29.08 | 6 |
| ATOM | 1342 | | 2 HIS A 170 | | 19.338 | 32.834 | | | |
| | | | | | | | 52.147 | 1.00 30.59 | 6 |
| MOTA | 1343 | | 1 HIS A 170 | | 20.384 | 33.995 | 53.675 | 1.00 30.77 | 7 |
| MOTA | 1344 | | 1 HIS A 170 | | 19.784 | 34.858 | 52.873 | 1.00 29.07 | 6 |
| MOTA | 1345 | NE: | 2 HIS A 170 | | 19.143 | 34.180 | 51.939 | 1.00 32.19 | 7 |
| ATOM | 1346 | С | HIS A 170 | | 20.895 | 30.113 | 55.958 | 1.00 26.00 | 6 |
| ATOM | 1347 | 0 | HIS A 170 | | 21.913 | 30.234 | 56.637 | 1.00 25.76 | 8 |
| ATOM | 1348 | N | HIS A 171 | | 20.349 | 28.939 | 55.658 | 1.00 27.29 | 7 |
| ATOM | 1349 | CA | HIS A 171 | | 20.893 | 27.655 | 56.090 | 1.00 25.01 | 6 |
| ATOM | 1350 | CB | HIS A 171 | | 19.934 | 26.532 | 55.663 | | |
| | 1351 | | | • | | | | 1.00 24.93 | 6 |
| MOTA | | CG | HIS A 171 | | 20.468 | 25.148 | 55.889 | 1.00 26.56 | 6 |
| MOTA | 1352 | | 2 HIS A 171 | | 20.674 | 24.123 | 55.028 | 1.00 22.34 | 6 |
| ATOM | 1353 | | l HIS A 171 | | 20.823 | 24.678 | 57.137 | 1.00 25.35 | 7 |
| MOTA | 1354 | CE1 | l HIS A 171 | | 21.222 | 23.424 | 57.036 | 1.00 22.68 | 6 |
| ATOM | 1355 | NEZ | 2 HIS A 171 | | 21.140 | 23.062 | 55.767 | 1.00 24.13 | 7 |
| MOTA | 1356 | С | HIS A 171 | | 22.267 | 27.413 | 55.471 | 1.00 24.74 | 6 |
| ATOM | 1357 | ō | HIS A 171 | | 22.540 | 27.863 | 54.356 | 1.00 28.22 | 8 |
| ATOM | 1358 | N | CYS A 172 | | 23.131 | 26.705 | | | |
| | | | | | | | 56.190 | 1.00 23.03 | 7 |
| ATOM | 1359 | CA | CYS A 172 | | 24.467 | 26.389 | 55.683 | 1.00 23.41 | 6 |
| ATOM | 1360 | CB | CYS A 172 | | 25.497 | 26.474 | 56.812 | 1.00 19.31 | 6 |
| MOTA | 1361 | SG | CYS A 172 | | 25.005 | 25.631 | 58.318 | 1.00 16.78 | 16 |
| ATOM | 1362 | С | CYS A 172 | | 24.484 | 24.997 | 55.048 | 1.00 25.45 | 6 |
| MOTA | 1363 | 0 | CYS A 172 | | 25.203 | 24.098 | 55.483 | 1.00 24.47 | 8 |
| MOTA | 1364 | N | ASP A 173 | | 23.664 | 24.839 | 54.015 | 1.00 26.67 | 7 |
| ATOM | 1365 | CA | ASP A 173 | | 23.542 | 23.593 | 53.269 | 1.00 26.47 | 6 |
| ATOM | 1366 | CB | ASP A 173 | | 22.735 | 23.857 | 51.993 | 1.00 26.33 | 6 |
| | 1367 | CG | ASP A 1'.3 | | 23.281 | 25.030 | | | |
| ATOM | | | | _ | | | 51.179 | 1.00 27.06 | 6 |
| ATOM | 1368 | | ASP A 173 | | 22.539 | 25.558 | 50.330 | 1.00 23.43 | 8 |
| MOTA | 1369 | | ASP A 173 | | 24.454 | 25.417 | 51.372 | 1.00 29.38 | 8 |
| MOTA | 1370 | С | ASP A 173 | | 24.872 | 22.932 | 52.922 | 1.00 26.65 | 6 |
| ATOM | 1371 | 0 | ASP A 173 | | 24.940 | 21.708 | 52.784 | 1.00 28.38 | 8 |
| ATOM | 1372 | N | GLY A 174 | | 25.926 | 23.737 | 52.793 | 1.00 25.24 | 7 |
| ATOM | 1373 | CA | GLY A 174 | | 27.227 | 23.198 | 52.447 | 1.00 23.11 | 6 |
| | 1374 | c | GLY A 174 | | | | | | |
| MOTA | | | | | 27.896 | 22.505 | 53.612 | 1.00 25.64 | 6 |
| ATOM | 1375 | 0 | GLY A 174 | | 28.443 | 21.408 | 53.462 | 1.00 27.67 | 8 |
| ATCM | 1376 | N | VAL A 175 | | 27.848 | 23.144 | 54.778 | 1.00 24.29 | 7 |
| MOTA | 1377 | CA | VAL A 175 | | 28.459 | 22.602 | 55.989 | 1.00 22.20 | 6 |
| ATOM | 1378 | CB | VAL A 175 | | 28.536 | 23.672 | 57.101 | 1.00 20.15 | 6 |
| MOTA | 1379 | CG1 | VAL A 175 | | 29.449 | 23.192 | 58.218 | 1.00 20.11 | 6 |
| ATOM | 1380 | | VAL A 175 | | 29.015 | 24.989 | 56.530 | 1.00 18.74 | 6 |
| ATOM | 1381 | c | VAL A 175 | | 27.647 | 21.409 | 56.505 | 1.00 22.85 | 6 |
| | | | | | | | | | 8 |
| ATOM | 1382 | 0 | VAL A 175 | | 28.173 | 20.512 | 57.173 | 1.00 20.07 | |
| ATOM | 1383 | N | GLN A 176 | | 26.356 | 21.404 | 56.203 | 1.00 24.12 | 7 |
| ATCM · | 1384 | CA | GLN A 176 | | 25.518 | 20.303 | 56. 62 9 | 1.00 27.18 | 6 |
| ATOM | 1385 | CB | GLN A 176 | | 24.045 | 20.611 | 56.355 | 1.00 32.86 | 6 |
| MOTA | 1386 | CG | GLN A 176 | | 23.084 | 19.483 | 56.726 | 1.00 36.04 | 6 |
| | | | | | | | - | | |

| ATOM | 138 | 37 (| D GLN A 176 | 21. | ควก | 19.862 |) 56 57. | | |
|--------------|--------------|----------|--------------------------|----------------|-----|------------------|------------------|--------------------------|--------|
| ATOM | | 38 (| E1 GLN A 176 | 21. | | 20.782 | | | 6 |
| ATOM | | | NE2 GLN A 176 | 20.9 | | 19.151 | | | |
| MOTA | | | GLN A 176 | 25.9 | | 19.083 | | | 7 |
| MOTA | | _ | | 26.3 | | 18.066 | | | |
| MOTA | | _ | | 25.9 | | 19.194 | | 1.00 28.89 | |
| ATOM | | | A GLU A 177 | 26.3 | | 18.062 | 53.698 | 1.00 27.96 | 7 |
| ATOM | | _ | B GLU A 177 | 26.3 | 395 | 18.460 | | | 6 |
| MOTA | | | G GLU A 177 | 26.3 | | 17.256 | | 1.00 36.20 | 6 |
| ATOM | | | D GLU A 177 | 26.2 | 273 | 17.626 | | 1.00 40.70 | 6 6 |
| ATOM | 139 | | E1 GLU A 177 | 27.3 | 22 | 17.967 | | 1.00 46.78 | |
| ATOM | 139 | | E2 GLU A 177 | 25.1 | 55 | 17.590 | | 40.70 | 8 8 |
| ATOM | 139 | _ | | 27.7 | | 17.516 | | 1.00 31.66 | 6 |
| MOTA | 140 | | | 27.8 | | 16.317 | | DE100 | 8 |
| ATOM ATOM | 140 | | | 28.6 | | 18.419 | | 1.00 33.39 | 7 |
| ATOM | 140 | | | 30.0 | | 18.072 | 54.673 | 1.00 31.63 | é |
| MOTA | 140: 140: | | | 30.8 | | 19.338 | | 1.00 30.96 | 6 |
| ATOM | 140 | | ALA A 178 | 30.2 | | 17.185 | 55.897 | 1.00 30.63 | 6 |
| ATOM | 140 | | ALA A 178 | 31.0 | | 16.276 | | 1.00 27.95 | 8 |
| ATOM | 140 | | PHE A 179 A PHE A 179 | 29.4 | | 17.444 | | 1.00 31.01 | 7 |
| MOTA | 1408 | | | 29.5 | | 16.656 | 58.184 | 1.00 31.34 | 6 |
| ATOM | 1409 | | | 30.1 | | 17.532 | | 1.00 30.13 | 6 |
| ATOM | 1410 | | | 31.18 30.8 | 89 | 18.505 | 58.858 | 1.00 27.78 | 6 |
| ATOM | 1411 | | | | | 19.790 | 58.466 | 1.00 28.24 | 6 |
| MOTA | 1412 | | | 32.5; 31.7 | | 18.124 | 58.766 | 1.00 28.33 | 6 |
| ATOM | 1413 | | | 33.48 | | 20.688 19.013 | 57.988 | 1.00 26.68 | 6 |
| ATOM | 1414 | CZ | | 33.13 | | 20.300 | 58.285 | 1.00 28.79 | 6 |
| ATOM | 1415 | C | PHE A 179 | 28.30 | | 16.003 | 57.895 | 1.00 28.67 | 6 |
| MOTA | 1416 | | PHE A 179 | 28.21 | | 15.542 | 58.664 59.803 | 1.00 32.06 | 6 |
| ATOM | 1417 | | TYR A 180 | 27.30 | | 15.960 | 57.787 | 1.00 30.58 | 8 |
| ATOM | 1418 | | | 26.00 | | 15.377 | 58.099 | 1.00 34.25 1.00 38.60 | 7 |
| MOTA | 1419 | | | 25.06 | | 15.605 | 56.911 | 1.00 38.99 | 6 |
| ATOM | 1420 | | TYR A 180. | 23.59 | 3 | 15:453 | 57.220 | 1.00 37.91 | 6 |
| ATOM | 1421 | | 1 TYR A 180 | 22.93 | 8 | 14.232 | 57.064 | 1.00 35.83 | 6 6 |
| ATOM | 1422 | CE | | 21.58 | 9 | 14.103 | 57.373 | 1.00 39.20 | 6 |
| ATOM ATOM | 1423 1424 | CD: | | 22.86 | | 16.543 | 57.694 | 1.00 37.56 | 6 |
| ATOM | 1425 | CE: | | 21.51 | | 16.430 | 58.007 | 1.00 40.28 | 6 |
| ATOM | 1426 | OH | TYR A 180 TYR A 180 | 20.88 | | 15.211 | 57.848 | 1.00 41.92 | 6 |
| ATOM | 1427 | C | TYR A 180 | 19.54 | | 15.110 | 58.188 | 1.00 43.41 | 8 |
| ATOM | 1428 | ō | TYR A 180 | 26.13 | | 13.884 | 58.382 | 1.00 40.28 | 6 |
| MOTA | 1429 | N | ASP A 181 | 25.15 | | 13.192 | 58.680 | 1.00 39.27 | 8 |
| ATOM | 1430 | CA | ASP A 181 | 27.36 27.63 | | 13.402 | 58.319 | 1.00 43.51 | 7 |
| ATOM | 1431 | CB | ASP A 181 | 28.41 | | 11.994 | 58.519 | 1.00 45.89 | 6 |
| ATOM | 1432 | CG | ASP A 181 | 28.83 | _ | 11.487 10.050 | 57.303 | 1.00 51.00 | 6 . |
| ATOM | 1433 | OD1 | | 29.63 | | 9.750 | 57.436 | 1.00 56.84 | 6 |
| MOTA | 1434 | OD2 | ASP A 181 | 28.34 | | 9.221 | 58.345 56.629 | 1.00 59.47 | 8 |
| MOTA | 1435 | С | ASP A 181 | 28.39 | | 11.665 | 59.804 | 1.00 60.73 1.00 44.75 | 8 |
| ATOM | 1436 | 0 | ASP A 181 | 28.25 | | 10.568 | 60.350 | 1.00 44.75 | 6 |
| ATOM | 1437 | N | THR A 182 | 29.194 | | 12.506 | 60.298 | 1.00 41.26 | 8 7 |
| MOTA | 1438 | CA | THR A 182 | 29.975 | | 12.337 | 61.495 | 1.00 39.51 | |
| ATOM | 1439 | CB | THR A 182 | 31.408 | 3 | 12.881 | 61.355 | 1.00 39.19 | 6 6 |
| MOTA | 1440 | OG1 | THR A 182 | 32.171 | L : | 12.508 | 62.505 | 1.00 37.82 | 8 |
| ATOM | 1441 | | THR A 182 | 31395 | 5 : | 14.397 | 61.232 | 1.00 40.12 | 6 |
| ATOM | 1442 | C | THR A 182 | 29.370 |) : | 12.910 | 62.759 | 1.00 38.58 | 6 |
| ATCM | 1443 | O | THR A 182 | 28.609 | | 13.876 | 62.716 | 1.00 41.24 | 8 |
| ATOM ATOM | 1444 | N | ASP A 183 | 29.712 | | 12.304 | 63.890 | 1.00 37.39 | 7 |
| MOTA MOTA | 1445 1446 | CA CB | ASP A 183 | 29.211 | _ | L2.773 | 65.171 | 1.00 39.24 | 6 |
| ATOM ATOM | 1447 | CB | ASP A 183 | 28.824 | - | 11.588 | 66.061 | 1.00 40.31 | 6 |
| ATOM | 1448 | | ASP A 183 ASP A 183 | 30.010 | _ | 10.723 | 66.433 | 1.00 41.64 | 6 |
| ATOM | 1449 | כמס | ASP A 183 ASP A 183 | 30.725 | | 10.268 | 65.520 | 1.00 42.53 | 8 |
| ATOM | 1450 | C | ASP A 183 | 30.221 | | 0.494 | 67.640 | 1.00 42.46 | 8 |
| ATOM | 1451 | ō | ASP A 183 | 30.286 | _ | 3,621 | 65.853 | 1.00 40.34 | 6 |
| TCM | 1452 | N | GLN A 184 | 30.109 | | 4.071 | 66.983 | 1.00 42.07 | 8 |
| | | | | 31.400 | 1 | 3.830 | 65.154 | 1.00 39.29 | 7 |

| ATOM | I 1453 CA GLN A 184 | 32.506 14.635 65.671 1 00 37 08 |
|-------|----------------------|--|
| ATOM | 1 1454 CB GLN A 184 | 22 020 00000 |
| ATOM | 1 1455 CG GLN A 184 | 42.00 33.// |
| ATOM | | 34.229 12.804 65.166 1.00 33.63 |
| | | 33.339 12.499 64.593 1.00 32 7% |
| ATOM | | 35 853 12 704 62 412 4 62 63 |
| MOTA | 1458 NE2 GLN A 184 | 25 400 31.1/ |
| ATOM | 1459 C GLN A 184 | 20 20 20 20 20 20 20 20 20 20 20 20 20 2 |
| ATOM | | 1.00 36.42 |
| | 1461 W 137 | 32.803 16.994 66.034 1.00 37.41 s |
| ATOM | | 31.329 16.372 64.456 1.00 33.14 |
| ATOM | | 30 004 17 740 64 440 |
| ATOM | | 31 300 10 053 50 544 |
| ATOM | 1464 CG1 VAL A 185 | 2.00 33.03 |
| ATOM | 1465 CG2 VAL A 185 | 20 25.27 |
| ATOM | | 32.773 17.738 62.357 1.00 34.58 |
| | | 29.508 17.972 64.360 1.00 31.51 6 |
| MOTA | | 40.000 17.124 64.038 1 00 31 71 0 |
| MOTA | 11 200 | 29 185 19 179 64 046 |
| ATOM | | 27 700 10 463 65 005 |
| ATOM | 1470 CB PHE A 186 | 27 524 19 532 66 716 1 00 31.44 6 |
| ATOM | 1471 CG PHE A 186 | 2000000 |
| ATOM | 1472 CD1 PHE A 186 | 26.059 19.617 67.066 1.00 31.59 6 |
| ATOM | 1472 CD1 PRE A 100 | 25.552 18.901 68.153 1.00 30.54 6 |
| | 1473 CD2 PHE A 186 | 25.179 20.395 66.308 1.00 31.50 6 |
| MOTA | 1474 CE1 PHE A 186 | |
| MOTA | 1475 CE2 PHE A 186 | 23 015 20 459 56 500 |
| MOTA | 1476 CZ PHE A 186 | 23 710 10 772 57 700 1.00 33.04 6 |
| ATOM | 1477 C PHE A 186 | 00 100 02.00 0 |
| ATOM | 1478 O PHE A 186 | 20 100 |
| ATOM | 1479 N VAL A 187 | +.00 JI.JZ 8 |
| ATOM | | 26.435 20.809 63.752 1.00 31.14 7 |
| MOTA | | 26.024 22.015 63.063 1.00 32 05 6 |
| | 1481 CB VAL A 187 | 26.018 21.805 61.525 1.00 33 54 6 |
| ATOM | 1482 CG1 VAL A 187 | 25 574 22 001 60 012 |
| ATOM | 1483 · CG2 VAL A 187 | 27 420 21 390 61 056 |
| MOTA | 1484 C VAL A 187 | |
| ATOM | 1485 O VAL A 187 | 23 566 21 505 52 410 |
| ATOM | 1486 N LEU A 188 | 23.00 |
| ATOM | 1487 CA LEU A 188 | 7.00 29.44 |
| ATOM | | 23.336 24.228 64.551 1.00 29.39 6 |
| ATOM | | 23.433 24.665 66.009 1.00 29.62 6 |
| | 1489 CG LEU A 188 | 22.293 25.589 66.458 1.00 27.92 6 |
| ATOM | 1490 CD1 LEU A 188 | 20.970 24.844 66.414 1.00 25.87 6 |
| MOTA | 1491 CD2 LEU A 188 | |
| MOTA | 1492 C LEU A 188 | 23 161 25 454 52 505 |
| MOTA | 1493 O LEU A 188 | 24 124 |
| MOTA | 1494 N SER A 189 | 2.00 31.30 8 |
| ATOM | 1495 CA SER A 189 | 21 500 7 |
| ATOM | 1496 CB SER A 189 | 21.682 26.831 62.390 1.00 24.65 6 |
| ATOM | | 21.873 26.411 60.942 1.00 22.40 6 |
| | | 21.585 27.485 60.083 1.00 19.12 8 |
| MOTA | 1498 C SER A 189 | 20.716 27.462 62.540 1.00 27.00 6 |
| ATOM | 1499 O SER A 189 | 1996 26.774 62.577 1.00 26.72 8 |
| MOTA | 1500 N LEU A 190 | 20 11 20 702 50 550 |
| ATOM | 1501 CA LEU A 190 | |
| ATOM | 1502 CB LEU A 190 | 2,00 25,00 |
| MOTA | 1503 CG LEU A 190 | 23.84 6 |
| ATOM | | 19.108 30.366 65.264 1.00 26.79 6 |
| | | 19.020 31.662 66.045 1.00 23.44 6 |
| ATOM | 1505 CD2 LEU A 190 | 17.881 29.549 65.546 1.00 27 63 6 |
| MOTA | 1506 C LEU A 190 | 19.046 30.141 61.329 1.00 29.58 6 |
| ATOM | 1507 O LEU A 190 | 20 004 20 505 50 555 |
| ATOM | 1508 N HIS A 191 | 17 064 33 32.40 8 |
| ATOM | 1509 CA HIS A 191 | 1.00 29.61 |
| MOTA | 1510 CB HIS A 191 | 22 23.72 0 |
| ATOM | | 18.595 29.839 58.432 1.00 26.47 6 |
| | | 18.225 28.392 58.504 1.00 28.18 6 |
| MOTA | 1512 CD2 HIS A 191 | 18.918 27.313 58.940 1.00 28.88 6 |
| ATOM | 1513 ND1 HIS A 191 | 16.989 27.921 58.118 1.00 31.00 7 |
| ATCM | 1514 CE1 HIS A 191 | 16.938 26.614 58.312 1.00 30.54 6 |
| ATOM | 1515 NE2 HIS A 191 | 10 000 00:011 00:012 1:00 00:04 0 |
| ATOM | 1516 C HIS A 191 | |
| ATOM | 1517 O HIS A 191 | |
| ATOM | 1518 N GLN A 192 | 00.322 02.333 2.00 27.81 0 |
| AION. | 10 N GLN A 132 | 16.183 31.346 57.649 1.00 29.39 7 |
| | • | • |

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1519
  MOTA
                 CA
                     GLN A 192
                                       14.886
                                               31.494
                                                        57.008
                                                                 1.00 28.21
  ATOM
          1520
                 CB
                     GLN A 192
                                       15.016
                                               32.416
                                                        55.796
                                                                  1.00 24.94
                                                                                6
  ATOM
          1521
                 CG
                     GLN A 192
                                      15.622
                                               33.773
                                                        56.124
                                                                  1.00
                                                                       21.66
                                                                                6
  ATOM
          1522
                 CD
                     GLN A 192
                                       15.701
                                               34.690
                                                        54.921
                                                                  1.00 22.22
                                                                                6
          1523
  ATOM
                 OE1
                     GLN A 192
                                                        54.428
                                       14.684
                                               35.173
                                                                 1.00 23.38
                                                                                8
  ATOM
          1524
                 NE2
                     GLN A 192
                                      16.914
                                               34.925
                                                        54.434
                                                                 1.00
                                                                       22.97
                                                                                7
  ATOM
          1525
                 C
                     GLN A 192
                                      14.435
                                               30.104
                                                        56.570
                                                                 1.00
                                                                      32.71
                                                                                6
          1526
  MOTA
                 O
                     GLN A 192
                                      15.157
                                                        55.853
                                               29.403
                                                                 1.00 33.85
                                                                                8
  ATOM
          1527
                 N
                     SER A 193
                                      13.249
                                               29.694
                                                        57.011
                                                                 1.00
                                                                       34.44
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  MOTA
          1528
                 CA
                     SER A 193
                                      12.751
                                               28.376
                                                        56.650
                                                                 1.00
                                                                       33.28
                                                                                6
  ATOM
          1529
                CB
                     SER A 193
                                      11.264
                                               28,249
                                                        56.961
                                                                 1.00
                                                                      33.25
                                                                                6
  ATOM
          1530
                OG
                     SER A 193
                                      10.786
                                               26.987
                                                        56.540
                                                                 1.00
                                                                       31.52
                                                                                8
  MOTA
          1531
                C
                     SER A 193
                                      12.974
                                               28.150
                                                        55.171
                                                                 1.00
                                                                      34.79
                                                                                6
  ATOM
          1532
                O
                     SER A 193
                                      12.775
                                               29.051
                                                        54.356
                                                                 1.00 33.74
                                                                                Я
  ATOM
          1533
                N
                     PRO A 194
                                      13.404
                                               26.938
                                                        54.803
                                                                 1.00
                                                                      37.57
                                                                                7
 ATOM
          1534
                CD
                     PRO A 194
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                                               25.775
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                                                                 1.00
                                                                      38.89
                                                                                6
         1535
  ATOM
                CA
                     PRO A 194
                                      13.654
                                               26.600
                                                        53.403
                                                                 1.00 37.81
                                                                                6
  ATOM
         1536
                CB
                     PRO A 194
                                      14.248
                                               25.194
                                                        53.498
                                                                 1.00
                                                                      39.30
                                                                                6
  ATOM
         1537
                CG
                     PRO A 194
                                      14.840
                                               25.163
                                                        54.916
                                                                 1.00 39.09
                                                                                6
  MOTA
         1538
                C
                     PRO A 194
                                                        52.638
                                      12.340
                                               26.617
                                                                 1.00 36.81
                                                                                6
 ATOM
         1539
                O
                     PRO A 194
                                      12.317
                                              26.443
                                                        51.425
                                                                 1.00
                                                                      34.09
                                                                                8
 MOTA
         1540
                N
                    GLU A 195
                                      11.246
                                              26.835
                                                        53.364
                                                                 1.00 39.25
                                                                                7
         1541
 ATOM
                CA
                    GLU A 195
                                       9.928
                                              26.866
                                                       52.750
                                                                 1.00 41.54
                                                                                6
 ATOM
         1542
                CB
                    GLU A 195
                                       8.843
                                              26.600
                                                       53.812
                                                                 1.00 45.84
                                                                               6
 ATOM
         1543
                CG
                    GLU A 195
                                       8.360
                                              27.811
                                                       54.608
                                                                 1.00 53.30
                                                                               6
 ATOM
         1544
                CD
                    GLU A 195
                                       7.160
                                              28.502
                                                       53.960
                                                                 1.00 55.91
                                                                               6
         1545
 MOTA
               OE1
                    GLU A 195
                                       6.735
                                              29.571
                                                       54.461
                                                                 1.00 55.14
                                                                               8
 MOTA
         1546
               OE2
                    GLU
                        A 195
                                       6.631
                                              27.966
                                                       52.956
                                                                 1.00 57.75
                                                                               8
 MOTA
         1547
               C
                    GLU A 195
                                      9.700
                                              28.208
                                                       52.047
                                                                 1.00 39.50
                                                                               6
 ATOM
         1548
               0
                    GLU A 195
                                      8.651
                                              28.431
                                                       51.452
                                                                 1.00
                                                                      40.21
                                                                               8
 ATOM
         1549
               N
                    TYR A 196
                                     10.689
                                              29.096
                                                       52.098
                                                                 1.00 37.13
                                                                               7
 ATOM
         1550
               CA
                    TYR A 196
                                     10.549
                                              30.379
                                                       51.434
                                                                 1.00
                                                                      35.50
                                                                               6
         1551
 ATOM
               CB
                    TYR A 196
                                      9.602
                                              31.274
                                                       52.245
                                                                1.00 36.36
                                                                               6
         1552
 MOTA
               CG
                    TYR A 196
                                     10.175
                                              31.816
                                                       53.538
                                                                1.00 37.28
 ATOM
         1553
               CD1
                    TYR A 196
                                     11.120
                                              32.848
                                                       53.527
                                                                1.00 35.42
                                                                               6
 ATOM
         1554
               CE1
                    TYR A 196
                                     11.637
                                              33.366
                                                       54.706
                                                                1.00
                                                                     33.10
                                                                               6
         1555
 ATOM
               CD2
                    TYR A 196
                                      9.764
                                              31.311
                                                       54.776
                                                                1.00 36.75
                                                                               6
         1556
 АТОМ
               CE2
                    TYR A 196
                                     10.279
                                              31.825
                                                       55.968
                                                                1.00
                                                                     35.26
 ATOM
        1557
               CZ
                    TYR A 196
                                     11.213
11.704
                                              32.856
                                                       55.922
                                                                1.00 35.84
                                                                               6
         1558
 ATOM
               OH
                    TYR A 196
                                              33.401
                                                       57.087
                                                                1.00 37.09
                                                                               8
        1559
 MOTA
               C
                    TYR A 196
                                     11.878
                                              31.097
                                                       51.188
                                                                1.00 34.89
                                                                               6
        1560
 ATOM
               O
                   TYR A 196
                                     11.896
                                              32.256
                                                       50.764
                                                                1.00 31.61
 ATOM
        1561
               N
                   ALA A 197
                                     12.991
                                             30.416
                                                       51.437
                                                                1.00
                                                                     34.39
                                                                               7
ATOM
        1562
               CA
                   ALA A 197
                                     14.297
                                                       51.242
                                             31.041
                                                                1.00 34.82
                                                                               6
ATOM
        1563
               CB
                   ALA A 197
                                     14.684
                                                      52.489
                                             31.826
                                                                1.00 32.48
ATOM
        1564
               C
                   ALA A 197
                                    15.418
                                             30.075
                                                      50.887
                                                                1.00 36.59
                                                                               6
ATOM
        1565
               0
                   ALA A 197
                                    15.407
                                             28.903
                                                      51.291
                                                                1.00 37.46
                                                                               8
ATOM
        1566
                   PHE A 198
              N
                                    16.388
                                             30.584
                                                      50.133
                                                                1.00 36.22
                                                                               7
ATOM
        1567
              CA
                   PHE A 198
                                    17.548
                                             29.802
                                                      49.722
                                                                1.00
                                                                     37.68
                                                                               6
ATOM
        1568
              CB
                   PHE A 198
                                    18.597
                                             30.729
                                                      49.109
                                                                1.00 40.89
                                                                               6
ATOM
        1569
              CG
                   PHE A 198
                                    19.810
                                             30.013
                                                      48.578
                                                                1.00 43.59
                                                                               6
ATOM
        1570
              CDI
                   PHE A 198
                                                      47.325
                                    19.783
                                             29.404
                                                               1.00 44.74
                                                                               6
                   PHE A 198
ATOM
        1571
              CD2
                                    20.970
                                             29.929
                                                      49.336
                                                               1.00 41.86
                                                                               6
ATOM
        1572
              CE1
                   PHE A 198
                                    20.894
                                                      46.833
                                                               1.00 41.42
                                             28.729
                                                                               6
              CE2
ATOM
        1573
                   PHE A 198
                                    22.079
                                                      48.849
                                             29.. 251
                                                               1.00 43.30
                                                                               6
MOTA
        1574
              CZ
                   PHE A 198
                                    22.040
                                                      47.595
                                                               1.00 41.86
                                             28.652
                                                                              6
ATOM
       1575
              С
                   PHE A 198
                                    18.139
                                             29.140
                                                      50.967
                                                               1.00
                                                                     37.00
                                                                              6
       1576
                                             29.754
ATOM
              0
                   PHE A 198
                                                      52.036
                                    18.166
                                                               1.00
                                                                     36.43
                                                                              8
       1577
              N
                   PRO A 199
MOTA
                                    18.641
                                                      50.848
                                                               1.00 37.63
                                             27.892
       1578
              CD
                   PRO A 199
ATOM
                                    19.298
                                                      51.997
                                             27.238
                                                               1.00
                                                                     35.29
                                                                              6
       1579
              CA
ATOM
                   PRO A 199
                                    18.727
                                             27.008
                                                      49.673
                                                               1.00
                                                                     36.52
                                                                              6
       1580
              CB
                   PRO A 199
MOTA
                                    19.702
                                                      50.138
                                             25.936
                                                               1.00 34.96
       1581
              CG
                  PRO A 199
ATOM
                                    19.281
                                                      51.565
                                             25.770
                                                               1.00 34.57
                                                                              б
              С
ATOM
       1582
                  PRO A 199
                                    17.409
                                                      49.222
                                                               1.00 35.72
                                             26.380
                                                                              6
       1583
ATOM
              0
                  PRO A 199
                                    17.386
                                                               1.00 37.36
                                            25.663
                                                      48.225
                                                                              8
             N
                  PHE A 200
       1584
ATOM
                                    16.331
                                                      49.962
                                                               1.00 33.78
                                             26.638
```

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Figure 17-25

| | | • |
|--------|---|-----------------------------------|
| ATC | M 1585 CA PHE A 200 | 15.004 26.090 49.662 1.00 32 15 6 |
| ATC | | 49.002 1.00 32.15 |
| ATO | | 10.222 1.00 28.39 6 |
| ATO | M 1588 CD1 PHE A 200 | 47.835 1.00 26.29 6 |
| ATO | | 47.296 1.00 24.82 6 |
| ATO | | 13.466 28.623 47.966 1.00 28.04 6 |
| | M 1501 CEI PHE A 200 | 15.767 29.712 46.882 1.00 25.68 6 |
| ATO | | 13.475 29 955 47 557 1 00 27 02 |
| ATO: | | 14.626 30.498 47.013 1.00 24.90 6 |
| ATO: | | 14 947 24 574: 40 042 1 22 |
| ATO | | 13 925 24 033 50 254 1 00 25.00 |
| ATO | M 1595 N GLU A 201 | 1.00 31.22 8 |
| ATO | M 1596 CA GLU A 201 | 16 129 22 420 40 505 |
| ATO | M 1597 CB GLU A 201 | |
| ATO | | 16 670 22 100 |
| ATO | | 16.879 22.182 47.175 1.00 33.52 6 |
| ATO | | 18.012 21.864 46.232 1.00 34.56 6 |
| ATON | | 18.396 20.678 46.117 1.00 36.35 8 |
| ATON | | 18.523 22.814 45.605 1.00 36.52 8 |
| ATOM | | 16.369 21.911 50.981 1.00 28.52 |
| | | 15.537 21.199 51.520 1 00 28 91 9 |
| 4OTA | | 17.511 22.239 51.566 1.00 31.64 7 |
| MOTA | 502 | 17.795 21.780 52.917 1.00 32.34 6 |
| MOTA | | 19 276 21 472 53 002 1 00 26 |
| ATOM | | 19 789 20 226 53 325 |
| ATOM | 202 | 20 212 20 500 50 001 1 00 |
| ATOM | | 20 952 10 428 50 028 |
| ATOM | 1610 NZ LYS A 202 | 21 504 10 002 40 005 |
| ATOM | 1611 C LYS A 202 | 17 421 22 242 57 |
| ATOM | 1612 O LYS A 202 | 16 977 27 999 57 596 |
| ATOM | 1613 N GLY A 203 | 17 710 22 571 55 200 1.00 20.35 8 |
| ATOM | 1614 CA GLY A 203 | 17 422 22 510 50.39 / |
| ATOM | 1615 C GLY A 203 | 16 016 |
| ATOM | 1616 O GLY A 203 | 1.00 23.23 6 |
| ATOM | 1617 N PHE A 204 | 15.915 23.975 58.041 1.00 32.90 8 |
| ATOM | 1618 CA PHE A 204 | 15.526 22.104 56.866 1.00 26.32 7 |
| ATOM | 1619 CB PHE A 204 | 14.344 21.779 57.657 1.00 23.25 6 |
| ATOM | | 13.366 20.917 56.863 1.00 21.25 6 |
| ATOM | 1620 CG PHE A 204 1621 CD1 PHE A 204 | 12.855 21.573 55.635 1.00 18.60 6 |
| ATOM | 1622 CD2 PHE A 204 | 13.605 21.560 54.461 1.00 16.43 6 |
| ATOM | | 11.654 22.273 55.664 1.00 14.82 6 |
| | | 13.168 22.245 53.333 1.00 16.91 6 |
| MOTA | 1624 CE2 PHE A 204 | 11.206 22.962 54.544 1.00 15.28 6 |
| ATOM | 1625 CZ PHE A 204 | 11.965 22.952 53.375 1.00 18.34 6 |
| ATOM | 1626 C PHE A 204 | 14.626 21.094 58.979 1.00 23.72 6 |
| ATOM | 1627 O PHE A 204 | 15.578 20.318 59.118 1.00 22.68 8 |
| MOTA | 1628 N LEU A 205 | 13.760 21.376 59.942 1.00 20.94 7 |
| MOTA | 1629 CA LEU A 205 | 13.877 20.818 61.272 1.00 24.83 6 |
| MOTA | 1630 CB LEU A 205 | 17 679 21 250 62 110 1 22 21 |
| MOTA | 1631 CG LEU A 205 | 12 672 20 021 : 2 500 |
| ATOM | 1632 CD1 LEU A 205 | 14 017 21 102 54 045 2 00 22 07 |
| ATOM | 1633 CD2 LEU A 205 | 11 479 31 456 64 855 |
| MOTA | 1634 C LEU A 205 | 1.00 20.02 |
| ATOM | 1635 O LEU A 205 | 14 443 19 770 62 210 1 00 00 70 |
| MOTA | 1636 N GLU A 206 | 13 635 10 600 |
| ATOM | 1637 CA GLU A 206 | 13 603 15 166 65 115 |
| ATOM | 1638 CB GLU A 206 | 12 776 |
| ATOM | 1639 CG GLU A 206 | 12.736 16.616 59.070 1.00 44.37 6 |
| ATOM | 1640 CD GLU A 206 | 11.284 17.060 59.204 1.00.50.75 6 |
| ATOM | 1641 OE1 GLU A 206 | 11.014 18.390 58.512 1.00 55.31 6 |
| ATOM | 1642 OE2 GLU A 206 | 9.9/2 19.027 58.797 1.00 55.36 8 |
| | | 11.839 18.786 57.661 1.00 56.48 8 |
| ATOM | | 13.114 16.674 59.847 1.00 40.00 6 |
| ATOM | 1644 O GLU A 206 | 15.483 15.541 60.180 1.00 39.35 g |
| ATOM · | 1645 N GLU A 207 | 15.903 17.536 59.217 1.00 39.38 7 |
| ATOM | 1646 CA GLU A 207 | 17.286 17.219 58.873 1.00 37.90 6 |
| MOTA | 1647 CB GLU A 207 | 17.776 18.242 57.854 1.00 37 36 6 |
| ATOM | 1648 CG GLU A 207 | 16.983 18.158 56.556 1.00 37.29 6 |
| ATOM | 1649 CD GLU A 207 | 16.978 19.452 55.773 1.00 38.16 6 |
| ATOM | 1650 OE1 GLU A 207 | 19 071 |
| | | 10.071 20.016 55.537 1.00 35.44 8 |
| | | |

| MOTA | | | E2 GLU | A 207 | 15.8 | 70 19.8 | 91 55.38 | 9 1.00 3 | 4.62 | 8 |
|--------|------|-----|-----------|--------|--------|----------|-----------|-----------|--------|-----|
| MOTA | 165 | 2 C | GĻU | A 207 | 18.1 | | | | | . 6 |
| ATOM | 165. | 3 0 | | A 207 | 18.5 | | | | | |
| ATOM | 165 | | | A 208 | | | | | | 8 |
| | | | | | 18.3 | | | | 4.45 | 7 |
| ATOM | 1655 | | | A 208 | 19.1 | 64 15.9 | 65 61.932 | 2 1.00 3 | 8.53 | 6 |
| MOTA | 1656 | 5 C | B ILE | A 208 | 18.2 | | | | | |
| ATOM | 1657 | 7 (| | A 208 | 19.0 | | | | | 6 |
| | 1658 | | | | | | | | | 6 |
| ATOM | | | 31 ILE | | 17.1 | 93 16.5 | 81 63.383 | 3 1.00 42 | 2.21 | 6 |
| MOTA | 1659 | CI | D1 ILE | A .208 | 16.2 | 91 16.2 | 86 64.560 | 1.00 4 | 4 . 81 | 6 |
| ATOM | 1660 |) C | ILE | A 208 | 20.4 | | | _ | | |
| ATOM | 1661 | | | A 208 | | _ | | | | 6 |
| | | | | | 21.2 | | | | | 8 |
| ATOM | 1662 | | | A 209 | 20.5 | 10 14.2 | 84 60.822 | 2 1.00 36 | 5.80 | 7 |
| ATOM | 1663 | CZ | A GLY | A 209 | 21.70 | 03 13.42 | 28 60.728 | 1.00 38 | 3.99 | 6 |
| MOTA | 1664 | С | GLY | A 209 | 21.5 | | | | | |
| ATOM | 1665 | | | A 209 | 20.4 | | | | | 6 |
| | 1666 | | | | | | | | | 8 |
| ATOM | | | | A 210 | 22.50 | | | | 2.16 | 7 |
| ATOM | 1667 | | GLU | A 210 | 22.49 | 2 10.18 | 35 58.930 | 1.00 43 | 1.30 | 6 |
| ATOM | 1668 | CE | GLU. | A 210 | 22.81 | 0 10.58 | | | | 6 |
| ATOM | 1669 | CG | | A 210 | 22.82 | | | | _ | |
| ATOM | 1670 | | | A 210 | | | | | | 6 |
| | | | | | 23.25 | | | | | 6 |
| ATOM | 1671 | | 1 GLU | A 210 | 24.41 | | 71 54.941 | 1.00 56 | .19 | 8 |
| MOTA | 1672 | OE | 2 GLU . | A 210 | 22.43 | 7 9.82 | 6 54.145 | 1.00 60 | 1.28 | 8 |
| MOTA | 1673 | С | GLU Z | A 210 | 23.58 | | | | | 6 |
| ATOM | 1674 | 0 | | A 210 | 24.75 | | | | | |
| ATOM | 1675 | N | | | | | | | | 8 |
| | | | | A 211 | 23.20 | | | 1.00 39 | .97 | 7 |
| ATOM | 1676 | CA | | | 24.18 | 1 7.40 | 60.885 | 1.00 37 | .34 | 6 |
| ATOM | 1677 | С | GLY A | A 211 | 24.64 | 2 7.95 | 2 62.224 | 1.00 37 | 84 | 6 |
| MOTA | 1678 | 0 | GLY A | A 211 | 23.82 | | | | | 8 |
| ATOM | 1679 | N | LYS A | | 25.94 | | | | | |
| ATOM | 1680 | CA | | | | • | | | | 7 |
| | | | | | 26.49 | | | | .29 | 6 |
| ATOM | 1681 | CB | LYS A | | 28.02 | 0 8.35 | 9 63.731 | 1.00 40 | .54 | 6 |
| ATOM | 1682 | CG | LYS A | | 28.57 | 0 6.95 | 0 63.675 | 1.00 46 | .39 | 6 |
| MOTA | 1683 | CD | LYS A | 1 212 | 28.14 | 9 6.14 | | | | 6 |
| ATOM | 1684 | CE | LYS A | | 28.55 | | | | | |
| ATOM | 1685 | NZ | LYS A | | | | | | | 6 |
| | • | | | | 30.03 | | | | | 7 |
| ATOM | 1686 | C | LYS A | | 26.06 | | 7 63.866 | 1.00 37 | . 68 | 6 |
| ATOM | 1687 | 0 | LYS A | 212 | 25.81 | 4 10.38 | 9 64.962 | 1.00 34 | .75 | 8 |
| ATOM | 1688 | N | GLY A | 213 | 25.95 | 6 10.57 | 4 62.728 | 1.00 38 | | 7 |
| ATOM | 1689 | CA | GLY A | 213 | 25.57 | | | 1.00 43 | | |
| MOTA | 1690 | C | GLY A | | | | | | | 6 |
| | | | | | 24.12 | | | 1.00 43 | | 6 |
| ATOM | 1691 | 0 | GLY A | | 23.73 | | 4 63.024 | 1.00 44 | . 67 | 8 |
| ATOM | 1692 | N | LYS A | 214 | 23.32 | 1 11.26 | 8 63.265 | 1.00 46 | . 02 | 7 |
| ATOM | 1693 | CA | LYS A | 214 | 21.90 | 7 11.46 | | 1.00 45 | | 6 |
| MOTA | 1694 | CB | LYS A | 214 | 21.16 | | | 1.00 47 | | |
| ATOM | 1695 | CG | LYS A | 21/ | | | | | | 6 |
| | 1696 | | | | 19.67 | | | 1.00 49 | | 6 |
| MOTA | | CD | LYS A | | 19.07 | | | 1.00 51 | .64 | 6 |
| ATOM · | 1697 | CE | LYS A | 214 | 17.63 | 7 9.03 | 8 62.440 | 1.00 54 | .30 | 6 |
| MOTA | 1698 | NZ | LYS A | 214 | 17.03 | 7.72 | 7 62.034 | 1.00 56 | .09 | 7 |
| ATOM | 1699 | С | LYS A | 214 | 21.80 | | | 1.00 44 | | 6 |
| MOTA | 1700 | 0 | LYS A | | 22.21 | | | | | |
| ATOM | 1701 | N | GLY A | | | | | 1.00 45 | | 8 |
| | | | | | 21.292 | | | 1.00 42 | . 89 | 7 |
| ATOM | 1702 | CA | GLY A | | 21.193 | 13.904 | | 1.00 40 | . 20 | 6 |
| ATOM | 1703 | С | GLY A | 215 | 22.295 | 14.931 | 1 66.600 | 1.00 39 | . 90 | 6 |
| MOTA | 1704 | 0 | GLY A | 215 | 22.356 | | | 1.00 40 | | 8 |
| ATOM | 1705 | N | TYR A | | 23.175 | | | | | |
| | | | | | | | | 1.00 38. | | 7 |
| ATOM | 1706 | CA | TYR A | | 24.261 | | 65.726 | 1.00 35. | . 91 | 6 |
| MOTA | 1707 | CB | TYR A | | 25.632 | 15.421 | 65.618 | 1.00 36. | . 47 | 6 |
| MOTA | 1708 | CG | TYR A | 216 | 25.935 | | | 1.00 39. | | 6 |
| MOTA | 1709 | | TYR A | 216 | 25.296 | | | 1.00 40. | | 6 |
| ATOM | 1710 | CEI | TYR A | 216 | | 3 | | | | |
| | | CDT | TIL N | 410 | 25.561 | | | 1.00 41. | | 6 |
| ATOM | 1711 | | TYR A | | 26.852 | 14.795 | 67.739 | 1.00 39. | .20 | 6 |
| MOTA | 1712 | CE2 | TYR A | 216 | 27.124 | | | 1.00 40. | | 6 |
| ATOM | 1713 | CZ | TYR A | | 26.475 | | | 1.00 41. | | 6 |
| ATOM | 1714 | OH | TYR A | | 26.743 | | | | | |
| | | | mvp » | 216 | | | | 1.00 43. | | 8 |
| ATOM | 1715 | C | TYR A | | 24.182 | | | 1.00 34. | | 6 |
| ATOM | 1716 | 0 | TYR A | 216 | 25.194 | 17.832 | 64.375 | 1.00 33. | 37 | 8 |
| | | • | | • • | | | - | • | | |
| | | • | P. 2 (10) | | | | | | | |

| ATO | M 1717 N ASNA 217 | 22.97 | 6 17 471 | 64 22 | | |
|-------|---------------------|--------|----------|--------|--------------|-----|
| ATO | | 22.72 | | | | • |
| . ATO | M 1719 CB ASN A 217 | 22.69 | | | | |
| ATO: | | | | | | . 6 |
| ATO | | 22.45 | | | | . 6 |
| ATO | | 21.35 | | | |) { |
| ATO | | 23.50 | | | 3 1.00 30.43 | |
| | | 21.36 | 9 19.116 | 63.645 | 1.00 29.09 | 6 |
| ATO | | 20.43 | | | 5 1.00 26.93 | à |
| ATO | | 21.26 | 3 20.440 | 63.710 | | 7 |
| ATO | | 20.010 | | | 1.00 25.33 | |
| ATOI | | 20.026 | | | 1.00 23.23 | |
| ATO | | 18.729 | | | 1.00 21.00 | 6 |
| OTA | | 19.100 | | 67.695 | | |
| ATO | | 17.872 | | 65.583 | | 6 |
| ATON | | 19.785 | | | | 6 |
| ATOM | | 20.596 | | | | 6 |
| ATOM | | 18.681 | | 63.415 | | 8 |
| ATOM | | 18.310 | | 62.584 | | 7 |
| ATOM | | | | 61.829 | 1.00 28.76 | 6 |
| ATOM | | 17.809 | | 60.417 | | 6 |
| ATOM | | 18.748 | | 59.646 | | 6 |
| ATOM | | 19.927 | | 59.505 | | 8 |
| ATOM | | 18.220 | | 59.114 | 20.57 | 7 |
| | | 17.129 | | 62.582 | 1.00 31.96 | 6 |
| ATOM | | 16.373 | 23.539 | 63.246 | 1.00 34.84 | 8 |
| ATOM | | 16.952 | 25.556 | 62.472 | 1.00 32.96 | 7 |
| MOTA | | 15.826 | 26.196 | 63.129 | 1.00 32.50 | 6 |
| MOTA | | 16.259 | 27.037 | 64.350 | 1.00 32.32 | 6 |
| MOTA | | 15.029 | 27.644 | 65.014 | 1.00 29.46 | 6 |
| ATOM | 1745 CG1 ILE A 220 | 16.978 | 26.160 | 65.374 | 1.00 29.65 | 6 |
| MOTA | 1746 CD1 ILE A 220 | 16.080 | 25.138 | 66.027 | 1.00 28.65 | 6 |
| MOTA | 1747 C ILE A 220 | 15.140 | 27.106 | 62.123 | 1.00 35.36 | 6 |
| MOTA | 1748 O ILE A 220 | 15.469 | 28.290 | 62.009 | 1.00 35.52 | 8 |
| ATOM | 1749 N PRO A 221 | 14.185 | 26.553 | 61.359 | 1.00 36.87 | 7 |
| MOTA | 1750 CD PRO A 221 . | 13.718 | 25.158 | 61.359 | 1.00 35.12 | 6 |
| ATOM | 1751 CA PRO A 221 | 13.445 | 27.318 | 60.356 | 1.00 35.41 | |
| ATOM | 1752 CB PRO A 221 | 12.509 | 26.262 | 59.767 | 1.00 35.68 | 6 |
| MOTA | 1753 CG PRO A 221 | 13.319 | 24.992 | 59.911 | 1.00 33.86 | 6 |
| ATOM | 1754 C PRO A 221 | 12.696 | 28.437 | 61.053 | 1.00 33.86 | 6 |
| ATOM | 1755 O PRO A 221 | 12.014 | 28.199 | 62.043 | | 6 |
| MOTA | 1756 N LEU A 222 | 12.815 | 29.655 | 60.547 | 1.00 38.79 | 8 |
| MOTA | 1757 CA LEU A 222 | 12.138 | 30.796 | 61.166 | 1.00 34.76 | 7 |
| ATOM | 1758 CB LEU A 222 | 13.173 | 31.735 | 61.798 | 1.00 33.87 | 6 |
| ATOM | 1759 CG LEU A 222 | 14.104 | 31.163 | | 1.00 35.13 | 6 |
| ATOM | 1760 CD1 LEU A 222 | 15.234 | 32.150 | 62.876 | 1.00 33.07 | 6 |
| ATOM | 1761 CD2 LEU A 222 | 13.312 | 30.856 | 63.154 | 1.00 34.04 | 6 |
| ATOM | 1762 C LEU A 222 | 11.287 | 31.567 | 64.141 | 1.00 32.39 | 6 |
| ATOM | 1763 O LEU A 222 | 11.669 | | 60.157 | 1.00 32.15 | 6 |
| ATOM | 1764 N PRO A 223 | 10.127 | 31.740 | 59.000 | 1. 0 31.32 | - 8 |
| MOTA | 1765 CD PRO A 223 | 9.606 | 32.060 | 60.601 | 1.17 30.97 | 7 |
| ATOM | 1766 CA PRO A 223 | | 31.913 | 61.972 | 1.00 32.34 | 6 |
| ATOM | 1767 CB PRO A 223 | 9.173 | 32.818 | 59.789 | 1.00 30.55 | 6 |
| ATOM | 1768 CG PRO A 223 | 7.957 | | 60.702 | 1.00 29.44 | 6 |
| ATOM | 1769 C PRO A 223 | 8.626 | | 62.046 | 1.00 31.02 | 6 |
| ATOM | | 9.645 | | 59.366 | 1.00 29.20 | 6 |
| | | 10.694 | | 59.796 | 1.00 31.95 | 8 |
| MOTA | | 8.841 | | 58.521 | 1.00 26.14 | 7 |
| ATOM | 1772 CA LYS A 224 | 9.115 | 36.172 | 58.026 | 1.00 23.54 | 6 |
| MOTA | 1773 CB LYS A 224 | 8.285 | | 56.766 | 1.00 24:71 | 6 |
| ATOM | 1774 CG LYS A 224 | | 35.500 | 55.619 | 1.00 23.83 | 6 |
| MOTA | 1775 CD LYS A 224 | 7.737 | | 54.394 | 1.00 20.59 | 6 |
| ATOM | 1776 CE LYS A 224 | 8.065 | | 53.329 | 1.00 27.03 | 6 |
| MOTA | 1777 NZ LYS A 224 | | | 52.122 | 1.00 30.48 | 7 |
| ATOM | 1778 C LYS A 224 | 8.702 | | 59.111 | 1.00 25.48 | 6 |
| ATOM | 1779 O LYS A 224 | | | 60.055 | 1.00 22.67 | 8 |
| ATOM | 1780 N GLY A 225 | | | 58.960 | 1.00 26.88 | 7 |
| ATOM | 1781 CA GLY A 225 | | | 9.925 | 1.00 29.80 | 6 |
| ATCM | 1782 C GLY A 225 | | | 51.286 | 1.00 32.96 | 6 |
| | | | | | 4.50 | • |
| | * | | | * | | • |

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| ATOM | 1783 | 0 | GLY | A 225 | | 9.068 | 39.861 | 62.271 | 1.00 | 31.20 | 8 |
|--------------|--------------|----------|--------|-------|---|------------------|------------------|------------------|-------|----------------|------------|
| MOTA | 1784 | N | LEU | A 226 | | 10.299 | 38.216 | 61.338 | | 32.86 | 7 |
| MOTA | 1785 | | | A 226 | | 10.975 | 37.877 | 62.575 | 1.00 | 34.55 | 6 |
| MOTA | 1786 | | | A 226 | | 12.149 | 36.958 | 62.255 | 1.00 | 34.46 | 6 |
| MOTA | 1787 | | | A 226 | | 12.982 | 36.413 | 63.407 | 1.00 | 34.48 | 6 |
| ATOM | 1788 | | LEU | | | 12.146 | 35.425 | 64.212 | | 33.18 | 6 |
| ATOM | 1789 | | LEU | | | 14.207 | 35.724 | 62.847 | 1.00 | 31.39 | 6 |
| MOTA | 1790 | | | A 226 | | 11.481 | 39.160 | 63.255 | | 36.29 | 6 |
| ATOM | 1791 | | | A 226 | | 12.156 | 39.970 | 62.613 | | 33.87 | 8 |
| ATOM | 1792 | | | A 227 | | 11.131 | 39.358 | 64.531 | | 37.31 | 7 |
| MOTA | 1793 | | | A 227 | - | 11.592 | 40.536 | 65.279 | | 37.26 | 6 |
| ATOM | 1794 1795 | | | A 227 | | 10.444 | 41.212 | 66.053 | | 35.57 | 6 |
| ATOM ATOM | 1796 | | ASN . | A 227 | | 9.920 | 40.368 | 67.208 | | 36.07 | 6 |
| ATOM | 1797 | | ASN . | | | 10.678 8.611 | 39.940 40.143 | 68.089 67.218 | | 35.08 | 8 |
| ATOM | 1798 | | | A 227 | | 12.688 | 40.143 | 66.259 | | 32.33 37.95 | 7 6 |
| ATOM | 1799 | | | A 227 | | 12.869 | 38.890 | 66.473 | | 37.08 | .8 |
| ATOM | 1800 | | | A 228 | | 13.403 | 41.063 | 66.832 | | 36.07 | 7 |
| ATOM | 1801 | CA | | A 228 | | 14.505 | 40.754 | 67.751 | | 37.63 | 6 |
| ATOM | 1802 | CB | | A 228 | | 14.996 | 42.007 | 68.486 | | 36.48 | |
| ATOM | 1803 | CG | | A 228 | | 15.480 | 43.088 | 67.545 | | 37.52 | 6 |
| ATOM | 1804 | OD1 | ASP A | A 228 | | 15.936 | 42.752 | 66.427 | | 35.28 | 8 |
| ATOM | 1805 | OD2 | ASP A | A 228 | | 15.426 | 44.274 | 67.937 | 1.00 | 39.01 | 8 |
| ATOM | 1806 | С | | A 228 | | 14.204 | 39.678 | 68.783 | 1.00 | 37.56 | 6 |
| MOTA | 1807 | 0 | | A 228 | | 14.921 | 38.678 | 68.869 | 1.00 | 39.53 | 8 |
| MOTA | 1808 | N | ASN A | | | 13.155 | 39.889 | 69.572 | | 38.37 | 7 |
| ATOM | 1809 | CA | ASN A | | | 12.766 | 38.935 | 70.605 | | 37.49 | 6 |
| MOTA | 1810 1811 | CB CG | ASN A | | | 11.422 | 39.352 | 71.200 | | 37.38 | 6 |
| ATOM ATOM | 1812 | | ASN A | | | 11.490 12.041 | 40.709 | 71.877 | | 40.47 | 6 |
| ATOM | 1813 | | ASN A | | | 10.960 | 40.840 41.735 | 72.973 71.212 | | 41.76 | 8 7 |
| ATOM | 1814 | C | ASN A | | | 12.680 | 37.530 | 70.017 | | 37.64 | 6 |
| ATOM | 1815 | ō | ASN A | | | 13.446 | 36.634 | 70.395 | | 35.76 | 8 |
| ATOM | 1816 | N | GLU A | | | 11.758 | 37.351 | 69.076 | | 36.01 | 7 |
| MOTA | 1817 | CA | GLU A | 230 | | 11.574 | 36.062 | 68.425 | | 34.74 | 6 |
| MOTA | 1818 | CB | GLU A | 230 | | 10.753 | 36.242 | 67.153 | 1.00 | 35.55 | 6 |
| ATOM | 1819 | CG | GLU A | | | 9.382 | 36.820 | 67.407 | 1.00 | 36.95 | 6 |
| ATOM | 1820 | CD | GLU A | | | 8.580 | 36.960 | 66.144 | | 35.30 | 6 |
| MOTA | 1821 | | GLU A | | | 9.042 | 37.670 | 65.229 | | 36.98 | 8 |
| ATOM | 1822 | | GLU A | | | 7.490 | 36.361 | 66.065 | | 36.71 | 8 |
| ATOM | 1823 1824 | С 0 | GLU A | | | 12.916 | 35.421 | 68.082 | | 33.92 | 6 |
| ATOM ATOM | 1825 | И | PHE A | | | 13.143 13.804 | 34.238 36.207 | 68.346 67.487 | | 32.74 32.03 | 8 7 |
| ATOM | 1826 | CA | PHE A | | | 15.116 | 35.712 | 67.123. | | 30.55 | 6 |
| ATOM | 1827 | CB | PHE A | | | 15.932 | 36.821 | 66.460 | | 33.86 | 6 |
| ATOM | 1828 | CG | HE A | | | 17.295 | 36.381 | 66.012 | | 36.97 | · 6 |
| ATOM | 1829 | CD1 | . HE A | 231 | | 17.438 | 35.334 | 65.102 | 1.00 | 40.41 | 6 |
| ATOM | 1830 | CD2 | .HE A | 231 | | 18.436 | 37.021 | 66.480 | 1.00 | 36.58 | 6 |
| MOTA | 1831 | | PHE A | | | 18.709 | 34.932 | 64.661 | 1.00 | 43.00 | 6 |
| ATOM | 1832 | | PHE A | | | 19.711 | 36.632 | 66.049 | | 39.07 | 6 |
| ATOM | 1833 | CZ | PHE A | | | 19.849 | 35.586 | | | 40.52 | 6 |
| ATOM | 1834 | C | PHE A | | | 15.835 | 35.232 | | .1.00 | | 6 |
| ATOM | 1835 | 0 | PHE A | | | 16.177 | 34.042 | 68.497 | | 29.66 | 8 |
| MOTA | 1836 | N | LEU A | | | 16.049 | 36.162 | 69.310 | | 24.94 | 7 |
| ATOM | 1837 1838 | CA CB | LEU A | | | 16.742 16.724 | 35.857 37.084 | 70.556 71.468 | | 22.82 24.96 | - 6 - 6 |
| ATOM ATOM | 1839 | | LEU A | | | 17.507 | 38.282 | 70.890 | | 29.34 | 6 |
| ATOM | 1840 | | LEU A | | | 17.316 | 39.549 | 71.746 | | 24.38 | 6 |
| ATOM | 1841 | | LEU A | | | 18.991 | 37.903 | 70.787 | | 27.39 | 6 |
| ATOM | 1842 | | LEU A | | | 16.150 | 34.638 | 71.261 | | 22.44 | 6 |
| ATOM | 1843 | | LEU A | | | 16.882 | 33.793 | 71.767 | | 20.37 | 8 |
| ATOM | 1844 | | PHE A | | | 14.825 | 34.552 | 71.289 | | 24.81 | 7 |
| MOTA | 1845 | CA | PHE A | 233 | | 14.131 | 33.422 | 71.905 | | 25.81 | 6 |
| ATOM | 1846 | CB | PHE A | 233 | | 12.623 | 33.535 | 71.641 | 1.00 | 24.37 | б |
| ATOM | 1847 | | PHE A | | | 11.811 | 32.373 | 72.157 | | 24.18 | 6 |
| ATOM | 1848 | CD1 | PHE A | 233 | | 11.491 | 32.264 | 73.503 | 1.00 | 25.59 | 6 |

| ATOM 1849 CD2 PHE A 233 ATOM 1850 CE1 PHE A 233 | 11.339 31.397 71.284 1.00 25.75 6 |
|---|--|
| ATOM 1851 CE2 PHE A 233 | 10.636 31.198 73.974 1.00 25.33 6 |
| ATOM 1852 CZ PHE A 233 | 10.548 30.327 71.747 1.00.24.02 6 |
| ATOM 1853 C PHE A 233 | 1, 66 |
| ATOM- 1854 O PHE A 233 | 15 00 20.04 6 |
| ATOM 1855 N ALA A 234 | 14 60. |
| ATOM 1856 CA ALA A 234 | 15,080 30,931 60,300 |
| ATOM 1857 CB ALA A 234 | 14.797 31 107 67 720 1.00 30.24 6 |
| ATOM 1858 C ALA A 234 | 16 563 30 645 60 422 1.00 33.38 6 |
| ATOM 1859 O ALA A 234 | 16.981 29 401 60 400 |
| ATOM 1860 N LEU A 235 | 17.363 31.695 69 563 1 00 37 04 |
| ATOM 1861 CA LEU A 235 | 18.789 31.486 69 790 1.00 32.02 |
| ATOM 1862 CB LEU A 235 ATOM 1863 CG LEU A 235 | 19.548 32.819 69.703 1.00 34.13 |
| | 21.039 32.745 69.316 1.00 36.32 |
| 101 210 A 2 33 | 21.625 34.156 69.205 1.00 36.44 |
| | 21.803 31.939 70.330 1.00 35 64 6 |
| | 18.970 30.846 71.176 1.00 30 75 6 |
| - 220 A 255 | 19.048 29.835 71.312 1.00 30 12 0 |
| ATOM 1868 N GLU A 236 ATOM 1869 CA GLU A 236 | 18.34/ 31.435 72.192 1.00 29 03 7 |
| ATOM 1870 CB GLU A 236 | 18.418 30.931 73.561 1.00 33 32 6 |
| ATOM 1871 CG GLU A 236 | 17.479 31.730 74.452 1.00 35.06 6 |
| ATOM 1872 CD GLU A 236 | 17.843 33.176 74.635 1.00 42.35 6 |
| ATOM 1873 OE1 GLU A 236 | 15.610 34.022 74.843 1.00 47.12 6 |
| ATOM 1874 OE2 GLU A 236 | 16 600 |
| ATOM 1875 C GLU A 236 | 17 000 |
| ATOM 1876 O GLU A 236 | 10 70 |
| ATOM 1877 N LYS A 237 | 16.767 29 250 77 176 1.00 30.43 8 |
| ATOM 1878 CA LYS A 237 | 15 100 33.0/ |
| ATOM 1879 CB LYS A 237 | 14.791 28 060 72 452 1 00 33.31 6 |
| ATOM 1880 CG LYS A 237 ATOM 1881 CD LYS A 237 | 13.745 27 022 72 045 |
| 11 231 | 12.712 27.605 73.821 1.00 40.66 6 |
| LL A 23/ | 13.312 28.054 75.153 1.00 40 58 6 |
| ATOM 1883 NZ LYS A 237 ATOM 1884 C LYS A 237 | 12.250 28.556 76.083 1.00 32.05 7 |
| ATOM 1885 O LYS A 237 | 17.025 26.891 72.485 1.00 35.07 6 |
| ATOM 1886 N SER A 238 | 17.315 25.833 73.061 1.00 30.60 8 |
| ATOM 1887 CA SER A 238 | 17.455 27.200 71.259 1.00 33.59 7 18.279 26.293 70.452 1.00 33.19 6 |
| ATOM 1888 CB SER A 238 | 10 4-5 |
| · ATOM 1889 OG SER A 238 | 10 0 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| ATOM 1890 C SER A 238 | 10 650 |
| ATOM 1891 O SER A 238 | 20 22 2 |
| ATOM 1892 N LEU A 239 | 20 357 35 300 71.00 20.88 8 |
| ATOM 1893 CA LEU A 239 | 21.660 26.650 72.147 1.00 30.63 |
| ATOM 1894 CB LEU A 239 ATOM 1895 CG LEU A 239 | 22.293 27.914 72.720 1.00 28 03 <i>5</i> |
| ATOM 1895 CG LEU A 239 ATOM 1896 CD1 LEU A 239 | 22.650 29.087 71.817 1.00 24 31 |
| ATOM 1897 CD2 LEU A 239 | 23.210 30.189 72.695 1 00 24 63 |
| ATOM 1898 C LEU A 239 | 23.663 28.681 70.770 1.00 23.11 6 |
| ATOM 1899 O LEU A 239 | 21.463 25.666 73.275 1.00 31.99 6 |
| ATOM 1900 N GLU A 240 | 22.279 24.764 73.473 1.00 32.57 8 |
| ATOM 1901 CA GLU A 240 | 20.367 25.835 74.009 1.00 33.86 7 |
| ATOM 1902 CB GLU A 240 | 20.094 24.965 75.136 1.00 38.61 6 18.799 25.369 75.842 1.00 43.21 |
| ATOM 1903 CG GLU A 240 | 10 50 |
| ATOM 1904 CD GLU A 240 | 19 677 24 363 78 655 |
| ATOM 1905 OE1 GLU A 240 | 10 051.505 70.022 1.00 36.39 6 |
| ATOM 1906 OE2 GLU A 240 | -51555 151701 1.00.37.81 8 |
| ATOM 1907 C GLU A 240 | 20 033 23 507 74 753 1.00 33.12 8 |
| ATOM 1908 O GLU A 240 | 20 532 22 622 75 122 1:00 39:28 6 |
| ATOM 1909 N ILE A 241 | 19.423 23.252 73.567 1.00.40.74 7 |
| ATOM 1910 CA ILE A 241 | 19.310 21.896 73.035 1.00 38.08 6 |
| ATOM 1911 CB ILE A 241 ATOM · 1912 CG2 ILE A 241 | 18.465 21.871 71.734 1.00 33.57 6 |
| | 18.536 20.506 71.086 1.00 31 39 6 |
| ATOM 1913 CG1 ILE A 241 ATOM 1914 CD1 ILE A 241 | 17.012 22.226 72.056 1.00 31.06 6 |
| A100 1914 CD1 ILE A 241 | 16.147 22.478 70.843 1.00 27.53 6 |
| | |

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| ATOM | 1919 | 5 C | ILE A 241 | | 20.713 | 21.372 | 72.747 | 1.00 39. | 56 6 |
|--------------|--------------|----------|-----------------------------|----|------------------|------------------|------------------|------------------------|-------------|
| MOTA | 1916 | | ILE A 241 | | 20.984 | 20.189 | 72.936 | 1.00 40. | |
| MOTA | 1917 | | VAL A 242 | | 21.605 | 22.254 | 72.299 | 1.00 41. | |
| MOTA | 1918 | | | | 22.979 | 21.842 | 72.015 | 1.00 45. | |
| MOTA | 1919 1920 | | 3 VAL A 242 31 VAL A 242 | | 23.808 | 22.959 | 71.329 | 1.00 45. | |
| ATOM ATOM | 1921 | | 2 VAL A 242 | | 25.242 23.182 | 22.479 | 71.116 | 1.00 43. | |
| ATOM | 1922 | | VAL A 242 | | 23.102 | 23.334 21.453 | 69.991 73.300 | 1.00 46. 1.00 45. | - |
| ATOM | 1923 | | VAL A 242 | | 24.191 | 20.331 | 73.423 | 1.00 46. | |
| ATOM | 1924 | | LYS A 243 | | 23.750 | 22.373 | 74.259 | 1.00 44. | |
| ATOM | 1925 | | | | 24.427 | 22.088 | 75.513 | 1.00 46. | |
| ATOM | 1926 | CE | LYS A 243 | | 24.214 | 23.217 | 76.527 | 1.00 49. | |
| ATOM | 1927 | | | | 25.061 | 23.023 | 77.795 | 1.00 54. | |
| ATOM | 1928 | | _ | | 24.652 | 23.934 | 78.939 | 1.00 58. | |
| ATOM | 1929 | | | | 24.782 | 25.399 | 78.577 | 1.00 64. | |
| ATOM | 1930 | | | | 24.274 | 26.283 | 79.676 | 1.00 66. | |
| ATOM ATOM | 1931 1932 | | LYS A 243 LYS A 243 | | 23.965 24.735 | 20.767 20.113 | 76.135 | 1.00 47. | |
| ATOM | 1933 | N | GLU A 244 | | 22.716 | 20.113 | 76.845 75.878 | 1.00 46 1.00 47. | |
| MOTA | 1934 | CA | | | 22.172 | 19.136 | 76.429 | 1.00 51. | |
| ATOM | 1935 | | | | 20.650 | 19.061 | 76.259 | 1.00 54. | |
| ATOM | 19,36 | CG | GLU A 244 | | 19.843 | 20.199 | 76.842 | 1.00 62. | |
| ATOM | 1937 | CD | _ | | 18.360 | 20.089 | 76.489 | 1.00 65. | |
| MOTA | 1938 | OE | | | 17,572 | 20.980 | 76.888 | | |
| ATOM | 1939 | OE: | | | 17.986 | 19.108 | 75.807 | 1.00 64. | |
| ATOM | 1940 1941 | С 0 | GLU A 244 GLU A 244 | | 22.745 | 17.936 | 75.698 | 1.00 50. | |
| ATOM ATOM | 1941 | N | VAL A 245 | | 22.866 23.104 | 16.846 18.148 | 76.259 74.441 | 1.00 51.9 | |
| ATOM | 1943 | CA | VAL A 245 | | 23.587 | 17.063 | 73.611 | 1.00 47. | |
| ATOM | 1944 | CB | VAL A 245 | | 2.704 | 16.980 | 72.336 | 1.00 48.4 | |
| ATOM | 1945 | | 1 VAL A 245 | | 3.082 | 15.765 | 71.499 | 1.00 51.6 | |
| ATOM | 1946 | | 2 VAL A 245 | | 21.226 | 16.934 | 72.731 | 1.00 45.0 | 55 6 |
| ATOM | 1947 | C | VAL A 245 | | 5.056 | 17.070 | 73.185 | 1.00 43.0 | |
| ATOM | 1948 | 0 | VAL A 245 | | 5.620 | 16.005 | 72.946 | 1.00 39.2 | |
| ATOM | 1949 1950 | N CA | PHE A 246 PHE A 246 | | 5.682 | 18.245 | 73.109 | 1.00 40.5 | |
| MOTA MOTA | 1951 | CB | PHE A 246 | | 7.063 7.023 | 18.321 18.700 | 72.633 71.154 | 1.00 38.5 | |
| ATOM | 1952 | CG | PHE A 246 | | 8.315 | 18.487 | 70.415 | 1.00 36.4 | |
| ATOM | 1953 | | PHE A 246 | | 8.749 | 17.201 | 70.098 | 1.00 32.9 | |
| ATOM | .1954 | CD2 | PHE A 246 | | 9.064 | 19.582 | 69.967 | 1.00 35.5 | |
| ATOM | 1955 | CEl | | | 9.903 | 17.004 | 69.337 | 1.00 33.8 | 30 G |
| MOTA | 1956 | CE2 | | | 0.222 | 19.397 | 69.206 | 1.00 34.4 | |
| ATOM | 1957 | cz | PHE A 246 | | 0.640 | 18.103 | 68.889 | 1.00 35.5 | |
| ATOM | 1958 1959 | С 0 | PHE A 246 PHE A 246 | | 7.970 7.613 | 19.311 | 73.371 | 1.00 40.8 | |
| atom Aota | 1960 | N | GLU A 247 | | 9.141 | 20.478 18.839 | 73.549 73.802 | 1.00 40.5 | |
| ATOM | 1961 | CA | GLU A 247 | | 0.128 | 19.695 | 74.467 | 1.00 43.9 | |
| ATOM | 1962 | CB | GLU A 247 | | 0.655 | 19.075 | 75.770 | 1.00 45.6 | - |
| ATOM | 1963 | CG | GLU A 247 | 2 | 9.763 | 19.243 | 77.005 | 1.00 51.6 | |
| MOTA | 1964 | CD | GLU A 247 | 2 | 8.478 | 18.424 | 76.962 | 1.00 57.4 | 2 6 |
| ATOM | 1965 | | GLU A 247 | | 7.645 | 18.644 | 76.058 | 1.00 62.1 | _ |
| MOTA | 1966 | OE2 | | | 8.296 | 17.557 | 77.845 | 1.00 59.4 | |
| ATOM | 1967 | С 0 | GLU A 247 GLU A 247 | | 1.268 | 19.839 | 73.464 | 1.00 43.6 | |
| ATOM · | 1968 1969 | N | PRO A 248 | | 2.077 1.342 | 18.931 20.988 | 73.294 72.780 | 1.00 44.2 1.00 43.6 | |
| atom atom | 1970 | CD | PRO A 248 | | 0.439 | 22.143 | 72.760 | 1.00 43.6 | |
| ATOM | 1971 | CA | PRO A 248 | | 2.371 | 21.260 | 71.779 | 1.00 43.2 | |
| ATOM | 1972 | CB | PRO A 248 | | 1.802 | 22.480 | 71.042 | 1.00 43.0 | |
| ATOM | 1973 | CG | PRO A 248 | | 3.317 | 22.474 | 71.415 | 1.00 43.0 | 26 |
| ATOM | 1974 | С | PRO A 248 | | 3.759 | 21.552 | 72.331 | 1.00 43.3 | 76 |
| ATOM | 1975 | 0 | PRO A 248 | | 3.896 | 22.286 | 73.305 | 1.00 45.4 | |
| ATOM | 1976 | N | GLU A 249 | | 1.788 | 20.982 | 71.710 | 1.00 42.3 | |
| ATOM | 1977 | CA | GLU A 249 | | 5.151 | 21.263 | 72.136 | 1.00 41.5 | |
| ATOM | 1978 | CB CG | GLU A 249 GLU A 249 | | 7.148 | 20.275 | 71.528 | 1.00 42.0 | |
| ATOM | 1979 1980 | CD | GLU A 249 | | 5.935 3.015 | 18.816 | 71.887 71.295 | 1.00 44.2 1.00 44.7 | |
| ATOM | T200 | | -mo w 747 | 20 | , | 17.908 | · · · 433 | 4.00 44./ | , , |

| ATOM | 1981 | OE1 GLU A 249 | 38.20 | 8 17.938 | 70.054 | 1.00 42.47 | 8 |
|-------|----------|---|----------------|----------------|------------------|--------------------------|--------|
| ATOM | 1982 | OE2 GLU A 249 | 38.66 | | | | 8 |
| ATOM | 1983 (| C GLU A 249 | 36.44 | | | | 6 |
| ATOM | 1984 (| O GLU A 249 | 37.15 | | | | 8 |
| ATOM | | VAL A 250 | 35.87 | | | | 7 |
| ATOM | | CA VAL A 250 | 36.05 | | | | 6 |
| ATOM | _ | CB VAL A 250 | 37.29 | | | | |
| ATOM | | G1 VAL A 250 | 37.12 | | | | 6 |
| ATOM | | G2 VAL A 250 | 37.48 | | | | 6 6 |
| ATOM | 1990 | | 34.83 | | | | |
| ATOM | | VAL A 250 | 34.16 | | | | 6 |
| ATOM | 1992 N | | 34.53 | | | | 8 |
| ATOM | | A TYR A 251 | 33.36 | | | | 7 |
| ATOM | | B TYR A 251 | 32.18 | | | | 6 |
| ATOM | | G TYR A 251 | 32.08 | | | | 6 |
| ATOM | | D1 TYR A 251 | 31.55 | | | | 6 |
| ATOM | | E1 TYR A 251 | 31.43 | | | 1.00 31.14 | 6 |
| ATOM | | D2 TYR A 251 | 32.49 | | 70.696 | 1.00 31.66 | 6 |
| ATOM | | | 32.38 | | 71.193 | | 6 |
| ATOM | | Z TYR A 251 | 31.854 | | | 1.00 33.89 | 6 |
| ATOM | | H TYR A 251 | 31.743 | | 70.391 70.867 | 1.00 34.75 | 6 |
| ATOM | 2002 C | - · · · · · · · · · · · · · · · · · · · | 33.570 | | 66.992 | 1.00 33.52 1.00 27.48 | 8 |
| ATOM | 2003 0 | | 34.167 | | 67.366 | | 6 |
| ATOM | - 2004 N | | 33.063 | | 65.773 | 1.00 24.78 | 8 |
| ATOM | 2005 C | | 33.150 | | 64.815 | 1.00 24.80 | 7 |
| ATOM. | 2006 C | | 33.631 | | 63.451 | | 6 |
| MOTA | 2007 C | | 35.126 | | 63.385 | 1.00 21.32 1.00 21.84 | 6 6 |
| ATOM | | D1 LEU A 252 | 35.457 | | 64.395 | 1.00 22.51 | |
| ATOM | | D2 LEU A 252 | 35.499 | | 61.986 | 1.00 22.07 | 6 6 |
| ATOM | 2010 C | LEU A 252 | 31.762 | | 64.729 | 1.00 22.56 | 6 |
| ATOM | 2011 0 | | 30.750 | | 64.856 | 1.00 21.99 | 8 |
| ATOM | 2012 N | | 31.734 | | 64.554 | 1.00 21.01 | 7 |
| ATOM | 2013 CZ | | 30.498 | | 64.461 | 1.00 18.89 | 6 |
| ATOM | 2014 CE | | 30.352 | | 65.695 | 1.00 20.05 | 6 |
| ATOM | 2015 CG | LEU A 253 | 29.198 | | 65.842 | 1.00 21.61 | 6 |
| ATOM | 2016 CI | D1 LEU A 253 | 27.849 | | 65.860 | 1.00 22.23 | 6 |
| MOTA | 2017 CI | 02 LEU A 253 | 29.395 | 33.716 | 67.145 | 1.00 22.90 | 6 |
| ATOM | 2018 C | LEU A 253 | 30.539 | 31.901 | 63.198 | 1.00 20.05 | 6 |
| ATOM | 2019 O | LEU A 253 | 31.466 | 32.691 | 62.987 | 1.00 18.17 | 8 |
| ATOM | 2020 N | GLN A 254 | 29.544 | 31.720 | 62.340 | 1.00 19.40 | 7 |
| MOTA | 2021 CA | GLN A 254 | 29.488 | 32.490 | 61.115 | 1.00 18.17 | 6 |
| MOTA | 2022 CB | | 29.017 | 31.592 | 59.969 | 1.00 9.67 | 6 |
| ATOM | 2023 CG | · | 27.584 | 31.713 | 59.601 | 1.00 18.43 | 6 |
| MOTA | 2024 CD | | 27.368 | 32.766 | 58.549 | 1.00 19.97 | 6 |
| ATOM | | 1 GLN A 254 | 27.917 | 32.677 | 57.450 | 1.00 22.54 | 8 |
| MOTA | | 2 GLN A 254 | 26.564 | 33.769 | 58.869 | 1.00 22.89 | 7 |
| ATOM | 2027 C | GLN A 254 | 28.520 | 33.634 | 61.444 | 1.00 19.75 | 6 |
| ATOM | 2028 0 | GLN A 254 | 27.470 | 33.415 | 62.060 | 1.00 18.77 | 8 |
| MOTA | 2029 N | LEU A 255 | 28.905 | 34.854 | 61.067 | 1.00 23.02 | 7 |
| ATOM | 2030 CA | LEU A 255 | 28.132 | 36.052 | 61.369 | 1.00 23.77 | 6 |
| ATOM | 2031 CB | LEU A 255 | 28.963 | 36.993 | 62.242 | 1.00 26.84 | 6 |
| MOTA | 2032 CG | LEU A 255 | 29.226 | 36.556 | 63.684 | 1.00 29.34 | 6 |
| ATOM | | 1 LEU A 255 | 30.196 | 37.520 | 64.331 | 1.00 30.65 | 6 |
| ATOM | | 2 LEU A 255 | 27.902 | 36.506 | 64.456 | 1.00 28.42 | 6 |
| ATOM | 2035 C | LEU A 255 | 27.605 | 36.842 | 60.197 | 1.00 24.84 | б |
| MOTA | 2036 O | LEU A 255 | 2 7.774 | 38.066 | 60.149 | 1.00 24.94 | 8 |
| ATOM | 2037 N | GLY A 256 | 26.969 | 36.158 | 59.254 | 1.00 25.07 | 7 |
| ATOM | 2038 CA | GLY A 256 | 26.408 | 36.858 | 58.117 | 1.00 26.11 | 6 |
| MOTA | 2039 C | GLY A 256 | 25.506 | 37.956 | 58.644 | 1.00 27.11 | 6 |
| ATOM | 2040 0 | GLY A 256 | 24.742 | 37.734 | 59.584 | 1.00 25.67 | 8 |
| ATOM | 2041 N | THR A 257 | 25.599 | 39.15 0 | 58.072 | 1.00 27.85 | 7 |
| MOTA | 2042 CA | THR A 257 | 24.757 | 40.244 | 58.536 | 1.00 29.28 | 6 |
| MOTA | 2043 CB | THR A 257 | 25.517 | 41.597 | 58.545 | 1.00 27.98 | 6 |
| ATOM | | THR A 257 | 26.002 | 41.895 | 57.232 | 1.00 31.91 | 8 |
| ATOM | 2045 CG2 | | 26.686 | 41.541 | 59.510 | 1.00 26.45 | 6 |
| MOTA | 2046 C | THR A 257 | 23.477 | 40.392 | 57.722 | 1.00 28.39 | 6 |
| | | | | | | | |

| ATOI | M 2047 O THR A 257 | 22.747 41.370 57 879 1 00 20 40 |
|------|---------------------|---|
| ATO | | 37.373 1.00 29.49 |
| ATON | | 23.192 39.414 56.867 1.00 29.13 |
| ATON | 1. 230 | 21.977 39.471 56.065 1.00 30.49 |
| ATO | 11 230 | 22.004 38.432 54.933 1.00 28.22 |
| ATOM | 11 250 | 22.337 37.033 55.416 1.00 29.39 |
| | 022 ASI A 236 | 21.893 36.653 56.520 1.00 30.16 |
| ATOM | 1.01 11 2.50 | 23.019 36 292 54 667 1 00 00 00 |
| ATOM | | |
| ATOM | I 2055 O ASP A 258 | 1.00 30.30 |
| ATOM | I 2056 N PRO A 259 | 1.00 32.07 |
| ATOM | 2057 CD PRO A 259 | 7. 7. 7. 7. 7. 7. 7. 7. 7. 7. 7. 7. 7. 7 |
| ATOM | 2058 CA PRO A 259 | 1.00 33.36 |
| MOTA | 223 | 19.366 38.821 58.806 1.00 31.73 |
| ATOM | | 19.705 37.912 59.987 1.00 31.87 |
| ATOM | :.0 11 233 | 21.067 38.373 60.333 1.00 31 73 |
| ATOM | | 18.81/ 40 184 50 260 2 00 20 00 |
| | | 1/ /36 40 270 50 045 3 44 44 |
| ATOM | | 19 565 41 745 50 000 1 10 20 10 |
| ATOM | | 19 161 42 592 50 275 1 00 29.38 |
| MOTA | 2065 CB LEU A 260 | 20.367 43 542 50 275 1 00 27 |
| MOTA | 2066 CG LEU A 260 | 1.00 2/.14 h |
| ATOM | 2067 CD1 LEU A 260 | 20 701 |
| ATOM | 2068 CD2 LEU A 260 | 53.002 1.00 13.79 6 |
| ATOM | 2069 C LEU A 260 | 01.00 10.25 6 |
| ATOM | 2070 O LEU A 260 | 17.992 43.165 58.576 1.00 28.09 6 |
| ATOM | | 1/./8/ 42.834 57.410 1.00 29.61 R |
| ATOM | | 1/.237 44.044 59.223 1 00 29 20 - |
| | | 16.097 44.693 58.596 1 00 29 71 6 |
| ATOM | 2073 CB LEU A 261 | 15 540 45 700 50 50 |
| ATOM | 2074 CG LEU A 261 | 14 405 45 664 50 050 |
| ATOM | 2075 CD1 LEU A 261 | 13 144 45 910 50 993 |
| ATOM | 2076 CD2 LEU A 261 | 14 170 47 050 50 000 |
| MOTA | 2077 C LEU A 261 | 16 461 45 333 57 353 |
| ATOM | 2078 O LEU A 261 | - 1200 23.30 8 |
| ATOM | 2079 N GLU A 262 | |
| ATOM | 2080 CA GLU A 262 . | 17.603 45.998 57.201 1.00 31.54 7 |
| ATOM | 2081 CB GLU A 252 | 18.015 46.664 55.973 1.00 31.93 6 |
| ATOM | 2082 CG GLU A 262 | 19.049 47.758 56 279 1 00 29 24 6 |
| ATOM | | 18.496 48.931 57.086 1.00 28.52 6 |
| | 2083 CD GLU A 262 | 18.449 48.687 58.589 1 00 29 76 |
| ATOM | 2084 OE1 GLU A 262 | 18.175 47.548 59.029 1.00 30.12 8 |
| ATOM | 2085 OE2 GLU A 262 | 19 661 40 661 50 500 |
| ATOM | 2086 C GLU A 262 | 19 526 45 254 54 255 |
| ATOM | 2087 O GLU A 262 | 10 600 46 100 71 |
| ATOM | 2088 N ASP A 263 | 10 770 |
| ATOM | 2089 CA ASP A 263 | 19 245 43 500 |
| ATOM | 2090 CB ASP A 263 | 20 354 40 570 |
| ATOM | 2091 CG ASP A 263 | 20 002 41 045 50 |
| ATOM | 2092 OD1 ASP A 263 | 22 25. |
| ATOM | 2093 OD2 ASP A 263 | 22.064 1.263 53.762 1.00 38.86 8 |
| ATOM | 2094 C ASP A 263 | 20.384 11.779 52.443 1.00 39.50 8 |
| ATOM | | 18.046 2.775 53.634 1.00 42.83 6 |
| | | 1/.4/4 41.966 54.381 1.00 44.22 8 |
| ATOM | 2096 N TYR A 264 | 17.673 43.002 52 377 1 00 44 14 7 |
| MOTA | 2097 CA TYR A 264 | 0 70X 47 757 51 706 1 00 46 00 00 |
| ATOM | 2098 CB TYR A 264 | 16 031 43 140 50 500 4 55 5 |
| atom | 2099 CG TYR A 264 | 2.00 34.01 |
| MOTA | 2100 CD1 TYR A 264 | 16 510 |
| ATOM | 2101 CE1 TYR A 264 | 17 220 |
| ATOM | 2102 CD2 TYR A 264 | 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| MOTA | 2103 CE2 TYR A 264 | 17.882 43.786 48.962 1.00 66.23 6 |
| | | 18.611 43.606 47.780 1.00 68.63 6 |
| | | 18.279 42.570 46.918 1.00 69.08 6 |
| | | 18.989 42.411 45.746 1.00 69.01 8 |
| | 2106 C TYR A 264 | 10.005 40 888 51 451 1 00 43 90 6 |
| | 2107 O TYR A 264 | 15.663 40.185 51.293 1.00 44.80 8 |
| | 2108 N LEU A 265 | 17.897 40.400 51.333 1.00 40.37 7 |
| | 2109 CA LEU A 265 | 10 000 |
| TCM | 2110 CB LEU A 265 | 1 2 30.303 31.010 2.00 38.08 0 |
| TOM | 2111 CG LEU A 265 | 10,010 |
| | 2112 CD1 LEU A 265 | |
| | | 21.176 38.535 48.703 1.00 26.97 6 |

| | 244 | | | | | | | | |
|--------|------|-----|-------------|---|--------|--------|--------------------------|------------|----|
| MOTA | 2113 | | | | 18.828 | 38.954 | 48.141 | 1.00 34.41 | 6 |
| MOTA | 2114 | | LEU A 265 | | 17.665 | 38.131 | 52.219 | 1.00 37.41 | 6 |
| MOTA | 2115 | 5 0 | LEU A 265 | | 18.125 | 37.000 | 52.370 | 1.00 37.96 | 8 |
| MOTA | 2116 | i N | SER A 266 | | 16.804 | 38.694 | | | 7 |
| MOTA | 2117 | | | | 16.294 | | | 1.00 36.46 | |
| ATOM . | | | | | | | | | 6 |
| | | | | | 17.263 | | | 1.00 37.22 | 6 |
| ATOM | 2119 | | | | 17.190 | | 55.991 | 1.00 37.41 | 8 |
| MOTA | 2120 |) C | SER A 266 | | 14.997 | 38.705 | 5 4 .6 5 3 | 1.00 35.55 | 6 |
| ATOM | 2121 | . 0 | SER A 266 | | 14.889 | 39.927 | 54.568 | 1.00 37.09 | 8 |
| ATOM | 2122 | N | LYS A 267 | | 14.018 | | | 1.00 34.33 | 7 |
| ATOM | 2123 | | | | 12.750 | | 55.532 | 1.00 36.13 | |
| ATOM | 2124 | | | | 11.596 | | | | 6 |
| • | | | | _ | | | 55.183 | 1.00 36.11 | 6 |
| MOTA | 2125 | | | | 11.503 | | 53.705 | | 6 |
| MOTA | 2126 | | LYS A 267 | | 11.453 | | 52.869 | 1.00 38.55 | 6 |
| ATOM_ | 2127 | CE | LYS A 267 | | 11.369 | 38.170 | 51.389 | 1.00 41.60 | 6 |
| ATOM | 2128 | NZ | LYS A 267 | | 11.503 | | 50.569 | 1.00 42.07 | 7. |
| MOTA | 2129 | | LYS A 267 | | 12.791 | | 57.043 | 1.00 34.90 | 6 |
| ATOM | 2130 | | LYS A 267 | | 11.758 | | | | |
| | | | | | | | 57.694 | 1.00 37.18 | 8 |
| ATOM | 2131 | N | PHE A 268 | | 13.998 | | 57.595 | 1.00 32.82 | 7 |
| ATOM | 2132 | CA | PHE A 268 | • | 14.192 | | 59.016 | 1.00 31.50 | 6 |
| ATOM | 2133 | CB | PHE A 268 | | 15.477 | 38.337 | 59.495 | 1.00 34.05 | 6 |
| ATOM | 2134 | CG | PHE A 268 | | 15.379 | 36.839 | 59.604 | 1.00 34.54 | 6. |
| MOTA | 2135 | ĆD: | L PHE A 268 | | 16.506 | | 59.940 | 1.00 35.04 | 6 |
| ATOM | 2136 | | PHE A 268 | | 14.161 | 36.178 | 59.429 | 1.00 34.57 | 6 |
| ATOM | 2137 | CE: | | | | | | | |
| | | | | | 16.423 | 34.691 | 60.108 | 1.00 35.44 | 6 |
| ATOM | 2138 | CE | | | 14.066 | 34.784 | 59.594 | 1.00 36.00 | 6 |
| MOTA | 2139 | CZ | PHE A 268 | | 15.201 | 34.040 | 59.936 | 1.00 34.68 | 6 |
| MOTA | 2140 | С | PHE A 268 | | 14.319 | 40.530 | 59.190 | 1.00 30.94 | 6 |
| ATOM | 2141 | 0 | PHE A 268 | | 14.983 | 41.192 | 58.394 | 1.00 30.27 | 8 |
| ATOM | 2142 | N | ASN A 269 | | 13.693 | 41.081 | 60.222 | 1.00 32.53 | 7 |
| ATOM | 2143 | CA | ASN A 269 | | 13.760 | 42.527 | 60.448 | 1.00 35.83 | 6 |
| ATOM | 2144 | CB | ASN A 269 | | 12.344 | 43.115 | | | |
| | | | | | | | 60.570 | 1.00 37.23 | 6 |
| ATOM | 2145 | CG | ASN A 269 | | 11.478 | 42.809 | - | 1.00 40.75 | 6 |
| MOTA | 2146 | | ASN A 269 | | 11.830 | 43.148 | 58.227 | 1.00 43.88 | 8 |
| MOTA | 2147 | ND2 | ASN A 269 | | 10.335 | 42.165 | 59.594 | 1.00 39.61 | 7 |
| ATOM | 2148 | С | ASN A 269 | | 14.553 | 42.854 | 61.710 | 1.00 35.45 | 6 |
| ATOM | 2149 | 0 | ASN A 269 | | 14.095 | 43.621 | 62.560 | 1.00 41.47 | 8 |
| ATOM | 2150 | N | LEU A 270 | | 15.747 | 42.285 | 61.827 | 1.00 33.27 | 7 |
| MOTA | 2151 | CA | LEU A 270 | | 16.571 | 42.510 | 63.004 | 1.00 30.68 | 6 |
| | 2152 | СВ | LEU A 270 | | | | | | |
| ATOM | | | | | 17.638 | 41.431 | 63.114 | 1.00 27.41 | 6 |
| MOTA | 2153 | CG | LEU A 270 | | 17.140 | 40.002 | 62.988 | 1.00 23.76 | 6 |
| MOTA | 2154 | | LEU A 270 | | 18.222 | 39.106 | 63.543 | 1.00 27.14 | 6 |
| ATOM | 2155 | CD2 | LEU A 270 | | 15.855 | 39.801 | 63.772 | 1.00 28.00 | 6 |
| ATOM | 2156 | C | LEU A 270 | | 17.258 | 43.856 | 63.033 | 1.00 32.30 | 6 |
| MOTA | 2157 | 0 | LEU A 270 | | 17.347 | 44.554 | 62.017 | 1.00 36.27 | 8 |
| ATOM | 2158 | N | SER A 271 | | 17.749 | 44.207 | 64.216 | 1.00 30.33 | 7 |
| ATOM | 2159 | CA | SER A 271 | | 18.465 | 45.457 | 64.424 | 1.00 30.79 | 6 |
| | 2160 | CB | SER A 271 | | | | | | |
| ATOM | | | | | 17.816 | 46.249 | 65.562 | 1.00 29.53 | 6 |
| MOTA | 2161 | OG | SER A 271 | | 17.712 | 45.471 | 66.739 | 1.00 30.43 | 8 |
| ATOM | 2162 | C | SER A 271 | | 19.911 | 45.109 | 64.768 | 1.00 33.09 | 6 |
| MOTA | 2163 | 0 | SER A 271 | | 20.194 | 43.972 | 65.172 | 1.00 29.64 | 8 |
| ATOM | 2164 | N | ASN A 272 | | 20.821 | 46.069 | 64.586 | 1.00 32.36 | 7 |
| ATOM | 2165 | CA | ASN A 272 | | 22.234 | 45.846 | 64.896 | 1.00 31.65 | 6 |
| ATOM | 2166 | CB | ASN A 272 | | 23.036 | 47.141 | 64.771 | 1.00 33.76 | 6 |
| | | | ASN A 272 | | | | 69.771 | | |
| MOTA | 2167 | CG | | | 23.101 | 47.658 | 63.361 | 1.00 37.76 | 6 |
| ATOM | 2168 | | ASN A 272 | | 23.719 | 48.686 | 63.100 | 1.00 36.12 | 8 |
| ATOM | 2169 | | ASN A 272 | | 22.460 | 46.952 | 62.437 | 1.00 44.79 | 7 |
| ATOM | 2170 | С | ASN A 272 | | 22.369 | 45.333 | 66.321 | 1.00 32.61 | 6 |
| ATOM | 2171 | 0 | ASN A 272 | | 22.970 | 44.283 | 66.565 | 1.00 27.95 | 8 |
| ATOM | 2172 | N | VAL A 273 | | 21.803 | 46.091 | 67.257 | 1.00 33.22 | 7 |
| | 2173 | | VAL A 273 | | 21.839 | 45.741 | 68.668 | 1.00 35.52 | 6 |
| ATOM | | | VAL A 273 | | 20.928 | | | | |
| ATOM | 2174 | | | | | 46.660 | 69.481 | 1.00 37.80 | 6 |
| ATCM | 2175 | | VAL A 273 | | 20.987 | 46.276 | 70.964 | 1.00 39.00 | 6 |
| ATOM · | 2176 | | VAL A 273 | | 21.356 | 48.112 | 69.275 | 1.00 38.88 | 6 |
| MOTA | 2177 | С | VAL A 273 | | 21.416 | 44.300 | 68.908 | 1.00 34.26 | 6 |
| ATOM | 2178 | 0 | VAL A 273 | | 22.060 | 43.580 | 69.679 | 1.00 35.96 | 8 |
| | | | | | | | _ | | |

| ATCM | 217 | 9 N | ALA A 274 | 20.32 | 8 43.88 | 0 60 26 | 3 3 3 3 3 3 3 3 3 | |
|--------------|--------------|------|------------------------|------------------|------------------|------------------|--------------------------|--------|
| ATCM | 218 | | | 19.83 | | | | |
| ATCM | 218 | 1 C | | 18.57 | | | | |
| ATCM | 218 | 2 C | | 20.92 | | | | |
| ATCM | | | | 21.32 | | | | |
| ATCM | 218 | 4 N | | 21.40 | | | | |
| ATOM | 218 | | | 22.46 | | | | |
| MOTA | 218 | | | 22.932 | | | | 6 |
| ATOM | 218 | | | 23.938 | | | | |
| ATCM | 218 | | D1 PHE A 275 | 23.597 | | | | |
| ATOM | 218 | | D2 PHE A 275 | 25.219 | | | | |
| MOTA | 219 | 0 C | E1 PHE A 275 | 24.513 | | | | 6 |
| MCTA | 219 | ı cı | E2 PHE A 275 | 26.149 | | | | |
| ATOM | 219 | | | 25.793 | | | | |
| MOTA | 2193 | 3 C | PHE A 275 | 23.632 | | | | 6 |
| ATOM | 2194 | 4 0 | PHE A 275 | 24.252 | | | | 6 |
| ATOM | 2195 | 5 N | LEU A 276 | 23.908 | | | | 8 |
| ATCM | 2196 | S CZ | LEU A 276 | 24.988 | | | 1.00 31.22 1.00 32.29 | 7 |
| ATOM | 2197 | 7 CE | LEU A 276 | 25.221 | | | 1.00 32.29 | 6 |
| ATOM | 2198 | 3 CG | LEU A 276 | 26.415 | | | 1.00 36.01 | 6 |
| ATOM | 2199 | CI | 1 LEU A 276 | 26.683 | | | | 6 |
| ATOM | 2200 |) CI | 2 LEU A 276 | 26.147 | | | | 6 |
| ATCM | 2201 | | LEU A 276 | 24.682 | | | | 6 6 |
| MOTA | 2202 | | LEU A 276 | 25.560 | | | 1.00 30.74 | 8 |
| ATOM | 2203 | | LYS A 277 | 23.445 | | | 1.00 33.95 | 7 |
| ATOM | 2204 | | | 23.086 | 40.413 | | 1.00 36.56 | 6 |
| ATOM | 2205 | | | 21.623 | 40.588 | 71.902 | 1.00 35.76 | 6 |
| ATOM | 2206 | | | 21.343 | 41.842 | | 1.00 42.31 | 6 |
| ATOM | 2207 | | | 20.743 | 41.508 | 74.049 | 1.00 45.72 | 6 |
| MOTA | 2208 | | LYS A 277 | 21.665 | 40.601 | 74.865 | 1.00 47.87 | 6 |
| MOTA | 2209 | | LYS A 277 | 21.140 | 40.378 | 76.244 | 1.00 44.36 | 7 |
| MOTA MOTA | 2210 2211 | | LYS A 277 | 23.302 | 38.974 | 71.092 | 1.00 37.98 | 6 |
| ATOM | 2211 | Ŋ | LYS A 277 | 23.875 | 38.179 | 71.845 | 1.00 37.54 | 8 |
| ATOM | 2213 | CA | ALA A 278 ALA A 278 | 22.832 | 38.654 | 69.886 | 1.00 37.17 | 7 |
| ATOM | 2214 | CB | ALA A 278 | 22.952 | 37.311 | 69.323 | 1.00 34.51 | 6 |
| ATOM | 2215 | c | ALA A 278 | 22.638 | 37.341 | 67.820 | 1.00 35.38 | 6 |
| ATOM | 2216 | ō | ALA A 278 | 24.368 24.605 | 36.831 35.790 | 69.550 | 1.00 30.63 | 6 |
| ATOM | 2217 | N | PHE A 279 | 25.303 | 37.624 | 70.167 | 1.00 27.62 | 8 |
| ATCM | 2218 | CA | PHE A 279 | 26.722 | 37.347 | 69.049 69.167 | 1.00 29.24 1.00 31.48 | 7 |
| ATOM | 2219 | CB | PHE A 279 | 27.490 | 38.558 | 68.645 | 1.00 31.48 | 6 6 |
| ATOM | 2220 | CG | PHE A 279 | 28.974 | 38.396 | 68.663 | 1.00 39.28 | 6 |
| ATCM | 2221 | CDI | PHE A 279 | 29.578 | 37.337 | 68.000 | 1.00 41.15 | 6 |
| MOTA | 2222 | CD2 | PHE A 279 | 29.776 | 39.328 | 69.315 | 1.00 40.66 | 6 |
| ATOM | 2223 | CE1 | | 30.960 | 37.209 | 67.987 | 1.00 44.22 | 6 |
| ATCM | 2224 | CE2 | | 31.153 | 39.213 | 69.378 | 1.00 41.38 | 6 |
| ATOM | 2225 | CZ | PHE A 279 | 31.750 | 38.152 | 68.614 | 1.00 44.52 | 6 |
| ATCM | 2226 | C | PHE A 279 | 27.116 | 37.043 | 70.€:1 | 1.00 31.81 | 6 |
| ATCM | 2227 | 0 | PHE A 279 | 27.627 | 35.953 | 70.935 | 1.00 27.51 | 8 |
| ATOM | 2228 | N | ASN A 280 | 26.860 | 38.005 | 71.503 | 1.00 29.32 | 7 |
| ATOM | 2229 2230 | CA | ASN A 280 | 27.192 | 37.851 | 72.907 | 1.00 29.26 | 6 |
| ATOM | | CB | ASN A 280 | 26.927 | 39.153 | 73.660 | 1.00 30.39 | 6 |
| ATOM | 2231 2232 | CG | ASN A 280 | 27.907 | 40.245 | 73.278 | 1.00 30.68 | 6 |
| atom Atom | 2232 | MD3 | ASN A 280 ASN A 280 | 29.117 | 40.030 | 73.303 | 1.00 33.34 | 8 |
| atom Atom | 2233 | C | | 27.395 | 41.419 | 72.931 | 1.00 27.00 | 7 |
| ATOM MCTA | 2235 | o | ASN A 280 ASN A 280 | 26.524 | 36.680 | 73.616 | 1.00 30.01 | 6 |
| atom Atom | 2235 | N | ILE A 281 | 27.167 | 36.004 | 74.419 | 1.00 29.58 | 8 |
| ATOM | 2237 | CA | ILE A 281 | 25.252 | 36.423 | 73.335 | 1.00 30.46 | 7 |
| ATOM | 2238 | CB | ILE A 281 | 24.594 | 35.291 | 73.983 | 1.00 33.71 | 6 |
| ATOM | 2239 | CG2 | ILE A 281 | 23.107 | 35.161 | 73.569 | 1.00 36.14 | 6 |
| etom etom | 2240 | CG1 | ILE A 281 | 22.541 22.298 | 33.820 | 74.032 | 1.00 36.18 | 6 |
| ATOM | 2241 | CD1 | ILE A 281 | 20.835 | 36.307 | 74.177 | 1.00 33.52 | 6 |
| TOM | 2242 | c | ILE A 281 | 25.330 | 36.243 | 73.834 | 1.00 37.16 | 6 |
| TOM | 2243 | ŏ | ILE A 281 | 25.385 | 34.006 33.071 | 73.631 74.437 | 1.00 34.06 1.00 31.94 | 6 |
| TOM | 2244 | N | VAL A 282 | 25.896 | 33.960 | 72.427 | 1.00 31.94 | 8 7 |
| | | | | | 33.300 | -4.441 | 1.00 33.31 | , |

| | | • | | | | |
|--------------|---------------------------------------|--------|--------|--------|--------------|----|
| ATOM | 1 2245 CA .VAL A 282 | 26.65 | 32.785 | 72.00 | = 1 00 36 4= | |
| ATOM | | 27.084 | | | | - |
| ATOM | | 27.829 | | 70.524 | | - |
| ATOM | | 25.880 | | | | |
| ATOM | | | | | | 6 |
| ATOM | | 27.919 | | 72.857 | | 6 |
| ATOM | | 28.182 | | | | |
| ATOM | | 28.693 | | | | 7 |
| | | 29.929 | | | 1.00 40.06 | 6 |
| ATOM | | 30.551 | | 73.449 | 1.00 39.38 | |
| ATOM | | 30.974 | 35.625 | 72.027 | | |
| MOTA | · · · · · · · · · · · · · · · · · · · | 31.492 | | 71.968 | 1.00 41.36 | 6 |
| MOTA | | 32.647 | 37.206 | 72.840 | | 7 |
| ATOM | | 33.162 | 38.373 | 73.215 | | 6 |
| MOTA | | 32.628 | | 72.797 | | 7 |
| ATOM | | 34.220 | | 74.014 | | 7 |
| MOTA | 2260 C ARG A 283 | 29.614 | | 75.044 | | 6 |
| ATOM | 2261 O ARG A 283 | 30.350 | 32.862 | 75.716 | | |
| ATOM | 2262 N GLUA 284 | 28.506 | 34.141 | 75.520 | | 8 |
| MOTA | 2263 CA GLU A 284 | 28.084 | 33.923 | 76.894 | | 7 |
| ATOM | 2264 CB GLU A 284 | 26.753 | 34.647 | 77.165 | | 6 |
| ATOM | 2265 CG GLU A 284 | 26.875 | 36.176 | 77.090 | | 6 |
| MOTA | 2266 CD GLU A 284 | 25.542 | 36.923 | | 1.00 56.10 | 6 |
| ATOM | 2267 OE1 GLU A 284 | 24.659 | | 77.179 | 1.00 60.77 | 6 |
| ATOM | 2268 OE2 GLU A 284 | 25.383 | 36.682 | 76.329 | 1.00 61.41 | 8 |
| ATOM | 2269 C GLU A 284 | 27.953 | 37.763 | 78.096 | 1.00 62.21 | 8 |
| ATOM | 2270 O GLU A 284 | 28.565 | 32.429 | 77.179 | 1.00 40.72 | 6 |
| ATOM | 2271 N VAL A 285 | 27.186 | 31.922 | 78.120 | 1.00 45.29 | 8 |
| ATOM | 2272 CA VAL A 285 | 26.975 | 31.721 | 76.354 | 1.00 34.82 | 7 |
| ATOM | 2273 CB VAL A 285 | | 30.288 | 76.551 | 1.00 30.84 | 6 |
| ATOM | 2274 CG1 VAL A 285 | 25.842 | 29.752 | 75.647 | 1.00 27.74 | 6 |
| ATOM | 2275 CG2 VAL A 285 | 25.698 | 28.253 | 75.831 | 1.00 22.95 | 6 |
| ATOM | 2276 C VAL A 285 | 24.545 | 30.433 | 75.982 | 1.00 26.26 | 6 |
| ATOM | 2277 O VAL A 285 | 28.181 | 29.366 | 76.341 | 1.00 31.93 | 6 |
| ATOM | 2278 N PHE A 286 | 28.492 | 28.556 | 77.214 | 1.00 33.46 | 8 |
| ATOM | 2279 CA PHE A 286 | 28.845 | 29.466 | 75.191 | 1.00 29.43 | 7 |
| ATOM | 2280 CB PHE A 286 | 29.973 | 28.586 | 74.907 | 1.00 24.26 | 6 |
| ATOM | 2281 CG PHE A 286 | 29.830 | 27.957 | 73.519 | 1.00 22.57 | 6 |
| ATOM | 2282 CD1 PHE A 286 | 28.607 | 27.095 | 73.345 | 1.00 23.46 | 6 |
| ATOM | 2283 CD2 PHE A 286 | 27.409 | 27.639 | 72.885 | 1.00 23.90 | 6 |
| ATOM | . 2284 CE1 PHE A 286 | 28.664 | 25.718 | 73.608 | 1.00 21.95 | 6 |
| ATOM | 2285 CE2 PHE A 286 | 26.281 | 26.814 | 72.681 | 1.00 24.90 | 6 |
| ATOM | 2286 CZ PHE A 286 | 27.547 | 24.892 | 73.411 | 1.00 18.06 | 6 |
| ATOM | | 26.357 | 25.437 | 72.945 | 1.00 20.23 | 6 |
| ATOM | | 31.368 | 29.200 | 74.991 | 1.00 25.14 | 6 |
| ATOM | | 32.338 | 28.566 | 74.560 | 1.00 23.16 | 8 |
| ATOM | | 31.480 | 30.416 | 75.525 | 1.00 25.51 | 7 |
| ATOM | | 32.783 | 31.065 | 75.614 | 1.00 26.86 | 6 |
| | | 33.353 | | 74.270 | 1.00 26.28 | 6 |
| MOTA MOTA | | 32.644 | 31.549 | 73.271 | 1.00 26.29 | 8 |
| | | 34.637 | 31.849 | 74.238 | 1.00 27.17 | 7 |
| MOTA | | 35.274 | 32.291 | 72.996 | 1.00 33.20 | 6 |
| ATOM | 2295 CB GLU A 288 | 36.680 | | 73.269 | 1.00 35.09 | 6 |
| ATOM | 3296 CG GLU A 288 | 36.726 | 34.104 | 74.083 | 1.00 41.67 | 6 |
| MOTA | 2297 CD GLU A 288 | 35.970 | 35.231 | 73.421 | 1.00 43.13 | 6 |
| MOTA | 3298 OE1 GLU A 288 | 36.221 | 35.493 | 72.228 | 1.00 45.39 | 8 |
| MOTA | 2299 OE2 GLU A 288 | 35.130 | 35.858 | 74.097 | 1.00 47.64 | 8 |
| MOTA | 2300 C GLU A 288 | | | 71.930 | 1.00 32.87 | 6 |
| MOTA | 2301 O GLU A 288 | 35.596 | | 72.247 | 1.00 31.59 | 8 |
| MOTA | 2302 N GLY A 289 | | | 70.668 | 1.00 31.93 | 7 |
| MOTA | 2303 CA GLY A 289 | | | 69.545 | 1.00 29.58 | 6 |
| MOT | 2304 C GLY A 289 | | _ | 68.307 | 1.00 27.42 | 5 |
| MOTA | 2305 O GLY A 289 | | | 68.398 | 1.00 26.27 | 8 |
| MOT | 2306 N VAL A 290 | | _ | 67.143 | 1.00 27.64 | 7 |
| MOT | 2307 CA VAL A 290 | | | 65.907 | 1.00 27.17 | 6 |
| MOT | 2308 CB VAL A 290 | | | 55.037 | 1.00 27.17 | 6 |
| MOT | 2309 CG1 VAL A 290 | | | | 1.00 23.23 | 6 |
| TOM | 2310 CG2 VAL A 290 | ' | | | 1.00 22.41 | 6 |
| | · - · · | | | 032 | 1.00 11.33 | ٠. |
| | | | | | | |

103/263 Figure 17-36

| ATOM | 2311 | С | VAL A 290 | 35.137 | 31.975 | 65.105 | 1.00 25.97 | 6 |
|-------|------|-----|--------------|------------------|--------|--------|------------|-----|
| ATOM | 2312 | ō | VAL A 290 | 34.218 | 31.279 | 64.672 | 1.00 22.32 | 8 |
| ATOM | 2313 | N | TYR A 291 | 35.217 | 33.293 | 64.914 | 1.00 27.33 | 7 |
| | 2314 | CA | | 34.188 | 34.052 | 64.203 | 1.00 26.69 | 6 |
| MOTA | | | | | | 64.939 | | |
| ATOM | 2315 | CB | | 33.925 | 35.356 | | 1.00 25.51 | 6 |
| MOTA | 2316 | CG | | 33.935 | 35.178 | 66.435 | 1.00 28.73 | 6 |
| ATOM | 2317 | | 1 TYR A 291 | 35.025 | 35.596 | 67.191 | 1.00 29.72 | 6 |
| ATOM | 2318 | | 1 TYR A 291 | | 35.414 | 68.563 | 1.00 29.53 | 6 |
| MOTA | 2319 | CD | 2 TYR A ·291 | 32.874 | 34.565 | 67.094 | 1.00 27.39 | 6 |
| MOTA | 2320 | CE | 2 TYR A 291 | 32.898 | 34.377 | 68.466 | 1.00 31.03 | 6 |
| ATOM | 2321 | CZ | TYR A 291 | - 33.997 | 34.808 | 69.194 | 1.00 31.85 | 6 |
| MOTA | 2322 | OH | TYR A 291 | 34.030 | 34.647 | 70.562 | 1.00 38.03 | 8 |
| MOTA | 2323 | С | TYR A 291 | 34.527 | 34.345 | 62.745 | 1.00 27.99 | 6 |
| ATOM | 2324 | - 0 | TYR A 291 | 35.608 | 34.843 | 62.415 | 1.00 24.83 | 8 |
| ATOM | 2325 | N | LEU A 292 | 33.567 | 34.042 | 61.880 | 1.00 30.17 | 7 |
| ATOM | 2326 | CA | LEU A 292 | 33.726 | 34.220 | 60.441 | 1.00 28.26 | 6 |
| ATOM | 2327 | | LEU A 292 | 33.561 | 32.861 | 59.741 | 1.00 27.70 | 6 |
| ATOM | 2328 | CG | LEU A 292 | 34.191 | 31.643 | 60.435 | 1.00 24.64 | 6 |
| | 2329 | | 1 LEU A 292 | 33.867 | 30.380 | 59.661 | 1.00 24.66 | 6 |
| ATOM | 2330 | | 2 LEU A 292 | 35.686 | 31.825 | 60.553 | 1.00 23.19 | |
| ATOM | 2331 | CD. | LEU A 292 | 32.649 | 35.175 | 59.944 | 1.00 25.59 | . 6 |
| ATOM | | | LEU A 292 | 31.640 | 35.394 | 60.611 | | |
| MOTA | 2332 | 0 | | | | 58.770 | 1.00 18.11 | 8 |
| ATOM | 2333 | N | GLY A 293 | 32.869 | 35.749 | | 1.00 28.55 | 7 |
| MOTA | 2334 | CA | GLY A 293 | 31.878 | 36.653 | 58.223 | 1.00 31.26 | 6 |
| ATOM' | 2335 | C | GLY A 293 | 30.722 | 35.815 | 57.714 | 1.00 34.84 | 6 |
| ATOM | 2336 | 0 | GLY A 293 | 30.463 | 34.724 | 58.234 | 1.00 34.11 | 8 |
| ATOM | 2337 | N | GLY A 294 | 30.036 | 36.312 | 56.689 | 1.00 35.34 | 7 |
| ATOM | 2338 | CA | GLY A 294 | • | 35.581 | 56.124 | 1.00 34.84 | 6 |
| MOTA | 2339 | С | GLY A 294 | 28.142 | 36.445 | 55.155 | 1.00 34.79 | 6 |
| ATOM | 2340 | 0 | GLY A 294 | 28.644 | 37.473 | 54.699 | 1.00 37.05 | 8 |
| MOTA | 2341 | N | GLY A 295 | 26.917 | 36.035 | 54.842 | 1.00 31.87 | 7 |
| MOTA | 2342 | CA | GLY A 295 | 26.102 | 36.806 | 53.925 | 1.00 27.78 | 6 |
| ATOM | 2343 | С | GLY A 295 | 25.969 | 38.245 | 54.378 | 1.00 27.09 | 6 |
| MOTA | 2344 | ,Ο | GLY A 295 | 26.192 | 38.558 | 55.546 | 1.00 27.03 | 8 |
| ATOM | 2345 | N | GLY A 296 | 25.596 | 39.119 | 53.450 | 1.00 24.67 | 7 |
| ATOM | 2346 | CA | GLY A 296 | 25.440 | 40.527 | 53.757 | 1.00 25.28 | 6 |
| ATOM | 2347 | С | GLY A 296 | 25.562 | 41.262 | 52.446 | 1.00 27.64 | 6 |
| ATOM | 2348 | 0 | GLY A 296 | 26.591 | 41.163 | 51.771 | 1.00 26.65 | 8 |
| ATOM | 2349 | N | TYR A 297 | 24.526 | 42.009 | 52.078 | 1.00 30.21 | 7 |
| ATOM | 2350 | CA | TYR A 297 | 24.543 | 42.704 | 50.801 | 1.00 30.62 | 6 |
| ATOM | 2351 | CB | TYR A 297 | 23.560 | 42.011 | 49.859 | 1.00 29.50 | 6 |
| ATOM | 2352 | CG | TYR A 297 | 23.717 | 40.516 | 49.953 | 1.00 30.33 | 6 |
| ATOM | 2353 | CD1 | TYR A 297 | 23.174 | 39.810 | 51.031 | 1.00 30.86 | 6 |
| MOTA | 2354 | CE1 | TYR A 297 | 23.450 | 38.449 | 51.226 | 1.00 30.74 | 6 |
| ATOM | 2355 | CD2 | TYR A 297 | 24.538 | 39.824 | 49.062 | 1.00 31.20 | 6 |
| ATOM | 2356 | CE2 | TYR A 297 | 24.821 | 38.460 | 49.247 | 1.00 32 08 | 6 |
| ATOM | 2357 | CZ | TYR A 297 | 24.275 | 37.781 | 50.332 | 1.00 30.92 | 6 |
| ATOM | 2358 | OH | TYR A 297 | 24.539 | 36.440 | 50.509 | 1.00 29 60 | 8 |
| ATOM | 2359 | С | TYR A 297 | 24.267 | 44.195 | 50.875 | 1.00 32.07 | 6 |
| ATOM | 2360 | o | TYR A 297 | 24.134 | 44.849 | 49.840 | 1.00 33.83 | 8 |
| ATOM | 2361 | N | HIS A 298 | 24.180 | 44.725 | 52.094 | 1.00 31.41 | 7 |
| ATOM | 2362 | CA | HIS A 298 | 23.961 | 46.153 | 52.289 | 1.00 33.94 | 6 |
| | 2363 | CB | HIS A 298 | 22.761 | 46.430 | 53.194 | 1.00 34.75 | 6 |
| MOTA | 2364 | CG | HIS A 298 | 22.379 | 47.880 | 53.256 | 1.00 35.16 | 6 |
| MOTA | 2365 | | HIS A 298 | 22.558 | 48.809 | 54.224 | 1.00 35.72 | 6 |
| MOTA | 2366 | | HIS A 298 | 21.779 | 48.538 | 52.205 | 1.00 34.10 | 7 |
| ATOM | | | HIS A 298 | 21.605 | 49.809 | 52.522 | 1.00 31.84 | 6 |
| ATOM | 2367 | NE2 | | | | 53.742 | 1.00 35.46 | 7 |
| ATOM | 2368 | | HIS A 298 | 22.069 25.213 | 50.000 | 52.962 | 1.00 36.21 | 6 |
| ATOM | 2369 | C | HIS A 298 | | 46.697 | 54.133 | 1.00 38.21 | 8 |
| ATOM | 2370 | 0 | | 25.471 | 46.405 | | 1.00 35.63 | |
| ATOM | 2371 | N | PRO A 299 | 25.992 | 47.519 | 52.234 | | 7 |
| ATOM | 2372 | CD | PRO A 299 | 25.680 | 47.997 | 50.881 | 1.00 35.57 | 6 |
| ATOM | 2373 | CA | PRO A 299 | 27.238 | 48.142 | 52.689 | 1.00 35.17 | 6 |
| ATOM | 2374 | CB | PRO A 299 | 27.586 | 49.073 | 51.525 | 1.00 37.75 | 6 |
| ATOM | 2375 | CG | PRO A 299 | 26.216 | 49.399 | 50.954 | 1:00 37.76 | 6 |
| ATOM | 2376 | C | PRO A 299 | 27.045 | 48.886 | 54.000 | 1.00 34.47 | 6 |

| ATO | 4 2377 O PRO A 299 | 27.78 | 1 48.67 | 0 54 06 | 3 2 20 22 44 | _ |
|--------------|---|------------------|---------------------------|---------|--------------|-----|
| MOTA | · | 26.05 | | | | |
| ATON | | 25.74 | | | | 9 7 |
| ATOM | | 24.49 | | | | 7 6 |
| ATOM | | 24.64 | | | | _ |
| ATOM | | 25.37 | | | | |
| ATOM | | 25.46 | | | | 6 |
| ATOM | | | | | | 6 |
| ATOM | | 24.01 | | | | |
| ATOM | | 24.09 | | | | - |
| ATOM | | 24.823 | | | | |
| ATOM | | 24.927 | | | | |
| ATOM | | 25.497 | | | | 6 |
| ATOM | | 26.062 | | | | 8 |
| ATOM | | 24.661 | | | | |
| ATOM | | 24.323 | | | 1.00 31.64 | |
| ATOM | | 23.216 | | | | |
| ATOM | | 25.539 | | | | |
| MOTA | | 25.848 | | | | 8 |
| ATOM | · · · · · · · · · · · · · · · · · · · | 26.223 | | | | 7 |
| ATOM | | 27.404 | | | | 6 |
| ATOM | | 28.012 | | | | 6 |
| ATOM | 2398 CG LEU A 302 2399 CD1 LEU A 302 | 29.315 | | | | 6 |
| ATOM | 2400 CD2 LEU A 302 | 29.491 | | 53.888 | | 6 |
| ATOM | 2400 CD2 LEU A 302 2401 C LEU A 302 | 30.475 | | | | 6 |
| ATOM | 2401 C LEU A 302 2402 O LEU A 302 | 28.418 | 46.136 | 57.663 | 1.00 29.79 | 6 |
| ATOM | | 28.796 | 45.676 | 58.746 | 1.00 27.68 | 8 |
| ATOM | | 28.842 | 47.299 | 57.179 | 1.00 27.92 | 7 |
| ATOM | | 29.818 | 48.119 | 57.877 | 1.00 25.00 | 6 |
| ATOM | 2405 CB ALA A 303 2406 C ALA A 303 | 30.026 | 49.424 | 57.137 | 1.00 23.62 | 6 |
| ATOM | 2407 O ALA A 303 | 29.397 | 48.397 | 59.305 | 1.00 25.06 | 6 |
| MOTA | 2407 0 ALA A 303 2408 N ARG A 304 | 30.088 | 48.015 | 60.248 | 1.00 26.90 | 8 |
| ATOM | 2400 K ARG A 304 2409 CA ARG A 304 | 28.258 | 49.054 | 59.472 | 1.00 24.06 | 7 |
| MOTA | 2410 CB ARG A 304 . | 27.794 | 49.382 | 60.810 | 1.00 24.37 | 6 |
| MOTA | 2410 CB ARG A 304 . | 26.420 | 50.052 | 60.758 | 1.00 23.99 | 6 |
| ATOM | 2412 CD ARG A 304 | 26.328 | 51.257 | 59.815 | 1.00 28.77 | 6 |
| ATOM | 2413 NE ARG A 304 | 25.106 | 52.089 | 60.156 | 1.00 29.96 | 6 |
| ATOM | 2414 CZ ARG A 304 | 23.943 22.893 | 51.233 | 60.369 | 1.00 36.43 | 7 |
| ATOM | 2415 NH1 ARG A 304 | 22.854 | 51.573 | 61.110 | 1.00 37.01 | 6 |
| ATOM | 2416 NH2 ARG A 304 | 21.896 | 52.757 | 61.713 | 1.00 36.37 | 7 |
| ATOM | 2417 C ARG A 304 | 27.727 | 50.719 48.142 | 61.269 | 1.00 34.36 | 7 |
| ATOM | 2418 O ARG A 304 | 28.343 | | 61.691 | 1.00 24.24 | 6 |
| ATOM | 2419 N ALA A 305 | 26.994 | 48.099 | 62.762 | 1.00 22.34 | 8 |
| ATOM | 2420 CA ALA A 305 | 26.801 | 47.132 | 61.221 | 1.00 24.51 | 7 |
| ATOM | 2421 CB ALA A 305 | 25.880 | 45.883 | 61.959 | 1.00 22.70 | 6 |
| ATOM | 2422 C ALA 305 | 28.089 | 44.960 | 61.175 | 1.00 18.13 | 6 . |
| ATOM | 2423 O ALA . 305 | 28.237 | 45.142 | 62.351 | 1.00 23.33 | . 6 |
| ATOM | 2424 N TRP 306 | 29.016 | 44.725 | 63.506 | 1.00 21.51 | 8 |
| ATOM | 2425 CA TRP A 306 | 30.244 | 44.961 | 61.411 | 1.00 22.79 | 7 |
| MOTA | 2426 CB TRP A 306 | 31.029 | 44.270 43.8 4 2 | 61.764 | 1.00 24.33 | 6 |
| MOTA | 2427 CG TRP A 306 | 30.604 | | 60.524 | 1.00 26.93 | 6 |
| ATOM | 2428 CD2 TRP A 306 | 30.861 | 42.503 | 59.952 | 1.00 27.96 | 6 |
| ATOM | 2429 CE2 TRP A 306 | 30.366 | 42.013 | 58.629 | 1.00 26.38 | 6 |
| ATOM | 2430 CE3 TRP A 306 | 31.462 | 40.688 | 58.570 | 1.00 24.96 | 6 . |
| ATOM | 2431 CD1 TRP A 306 | | 42.563 | 57.490 | 1.00 23.00 | 6 |
| ATOM | 2432 NE1 TRP A 306 | 29.983 | 41.484 | 60.620 | 1.00 28.53 | 6 |
| ATOM | 2433 CZ2 TRP A 306 | 29.837 | 40.392 | 59.797 | 1.00 25.62 | 7 |
| ATOM | 2434 CZ3 TRP A 306 | 30.450 31.548 | 39.904 | 57.414 | 1.00 24.51 | 6 |
| ATOM ATOM | 2435 CH2 TRP A 306 | 31 040 | 41.784 | 56.343 | 1.00 25.37 | 6 |
| ATOM | 2436 C TRP A 306 | 31.042 | 40.465 | 56.315 | 1.00 24.20 | 6 |
| ATOM | 2437 O TRP A 306 | 31.129 | 45.108 | 62.676 | 1.00 26.51 | 6 |
| ATOM ATOM | 2437 O TRP A 300 2438 N THR A 307 | 31.908 | 44.570 | 63.464 | 1.00 25.07 | 8 |
| ATOM | 2439 CA THR A 307 | | 46.427 | 62.575 | 1.00 28.08 | 7 |
| | 2440 CB THR A 307 | | 47.323 | 63.415 | 1.00 27.91 | 6. |
| ATOM | 2441 OG1 THR A 307 | | 48.796 | 63.100 | 1.00 27.86 | 6 |
| | 2441 OG1 THR A 307 | | 49.119 | 61.799 | 1.00 30.17 | 8 |
| ATOM | Lare COS INK N 307 | 32.120 | 49.704 | 64.137 | 1.00 24.72 | 6 |
| | | | | | • | _ |

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Figure 17-38

| ATOM | 244 | 3 C | THR A 30 | 7 | 31.44 | 1 47.041 | 64.863 | 3 1.00 29.35 | 6 |
|-------|------|----------|---------------------|---|----------|----------|--------|--------------|----|
| ATOM | 244 | 4 0 | THR A 30 | , | 32.316 | | | | |
| ATOM | 244 | 5 N | | | 30.159 | | | | _ |
| MOTA | | | | | | | | ~ | |
| ATOM | | | | | 29.740 | | | | |
| | | | DEU A 300 | , | 28.256 | | | | |
| ATOM | 244 | | | | 27.338 | | 66.058 | 3 1.00 34.79 | 6 |
| MOTA | | | D1 LEU A 308 | | 25.903 | 46.887 | 66.153 | | |
| MOTA | 2450 | 0 C | D2 LEU A 308 | | 27.569 | 48.542 | | | |
| ATOM | 2453 | l C | LEU A 308 | | 30.531 | 45.353 | | 1.00 34.57 | |
| ATOM | 2452 | 2 0 | LEU A 308 | | 31.230 | | | | |
| ATOM | 2453 | | ILE A 309 | | | | | | |
| ATOM | 2454 | | | | . 30.423 | | | | |
| | | | | | 31.108 | | | | 6 |
| ATOM | 2455 | | | | 30.939 | | | | 6 |
| MOTA | 2456 | | 32 ILE A 309 | | 31.733 | | 65.799 | 1.00 31.21 | 6 |
| MOTA | 2457 | | 31 ILE A 309 | | 29.445 | 41.631 | | | 6 |
| ATOM | 2458 | CI CI | D1 ILE A 309 | | 28.726 | | | | 6 |
| ATOM | 2459 |) C | ILE A 309 | | 32.589 | | | | |
| ATOM | 2460 | 0 | ILE A 309 | | 33.183 | 42.617 | _ | | 6 |
| ATOM | 2461 | | TRP A 310 | | | 44 111 | | | 8 |
| ATOM | 2462 | | | | 33.197 | | 65.977 | | |
| | | | | | 34.612 | | 66.169 | | 6 |
| MOTA | 2463 | | | | 35.150 | 45.311 | 65.075 | 1.00 32.61 | 6 |
| ATOM | 2464 | | | | 36.619 | 45.588 | 65.220 | 1.00 30.79 | 6 |
| MOTA | 2465 | CE | | | 37.679 | 44.620 | 65.274 | | 6 |
| MOTA | 2466 | CE | 2 TRP A 310 | | 38.882 | 45.330 | 65.474 | 1.00 28.42 | 6 |
| ATOM | 2467 | CE | | | 37.731 | 43.224 | 65:174 | 1.00 31.59 | |
| MOTA | 2468 | CD | | | 37.206 | 46.804 | 65.380 | | 6 |
| ATOM | 2469 | | | | 38.565 | 46.659 | | 1.00 30.62 | 6 |
| ATOM | 2470 | | | | 40.126 | | 65.536 | 1.00 29.37 | 7 |
| ATOM | 2471 | CZ | | | | 44.691 | 65.578 | 1.00 27.91 | 6 |
| | 2472 | CH | | | 38.978 | 42.585 | 65.279 | 1.00 28.06 | 6 |
| ATOM- | | | | | 40.150 | 43.322 | 65.479 | 1.00 26.50 | 6 |
| ATOM | 2473 | C | TRP A 310 | | 34.744 | 45.040 | 67.545 | 1.00 36.00 | 6 |
| MOTA | 2474 | 0 | TRP A 310 | | 35.365 | 44.476 | 68.440 | 1.00 36.24 | 8 |
| MOTA | 2475 | N | CYS A 311 | | 34.134 | 46.213 | 67.715 | 1.00 34.57 | 7 |
| ATOM | 2476 | ÇA | CYS A 311 | | 34.183 | 46.937 | 68.985 | 1.00 32.82 | 6 |
| ATOM | 2477 | CB | CYS A 311 | | 33.169 | 48.085 | 68.996 | 1.00 35.62 | 6 |
| ATOM | 2478 | SG | CYS A 311 | | 33.439 | 49.401 | 67.796 | 1.00 32.36 | |
| ATOM | 2479 | C | CYS A 311 | | 33.912 | 46.061 | | | 16 |
| ATOM | 2480 | ō | CYS A 311 | | 34.452 | | 70.206 | 1.00 32.01 | 6 |
| ATOM | 2481 | N | GLU A 312 | | | 46.313 | 71.280 | 1.00 29.82 | 8 |
| ATOM | 2482 | CA | | | 33.062 | 45.049 | 70.053 | 1.00 32.57 | 7 |
| | | | GLU A 312 | | 32.731 | 44.159 | 71.171 | 1.00 33.86 | 6 |
| ATOM | 2483 | CB | GLU A 312 | | 31.557 | 43.252 | 70.807 | 1.00 34.19 | 6 |
| ATCM | 2484 | CG | GLU A 312 | | 30.442 | 43.185 | 71.844 | 1.00 40.27 | 6 |
| ATOM | 2485 | CD | GLU A 312 | | 30.923 | 42.821 | 73.239 | 1.00 43.80 | 6 |
| ATOM | 2486 | OE: | GLU A 312 | | 31.685 | 41.831 | 73.383 | 1.00 44.81 | 8 |
| ATOM | 2487 | OE2 | 2 GLU A 312 | | 30.516 | 43.522 | 74.195 | 1.00 41.54 | 8 |
| ATOM | 2488 | C | GLU A 312 | | 33.953 | 43.298 | 71.456 | 1.00 33.77 | 6 |
| ATOM | 2489 | 0 | GLU A 312 | | 34.253 | 42.957 | 72.603 | 1.00 32.07 | 8 |
| ATOM | 2490 | N | LEU A 313 | | 34.647 | 42.945 | 70.382 | | |
| ATOM | 2491 | CA | LEU A 313 | | 35.848 | | | 1.00 33.45 | 7 |
| ATOM | 2492 | CB | LEU A 313 | | | 42.135 | 70.473 | 1.00 32.89 | 6 |
| | | | | | 36.172 | 41.513 | 69.115 | 1.00 32.14 | 6 |
| ATOM | 2493 | CG | LEU A 313 | | 35.154 | 40.493 | 68.626 | 1.00 27.73 | 6 |
| ATCM | 2494 | CDI | LEU A 313 | | 35.587 | 39.956 | 67.269 | .1.00 30.39 | 6 |
| ATCM | 2495 | | LEU A 313 | | 35.053 | 39.367 | 69.648 | 1.00 27.87 | 6 |
| ATOM | 2496 | C | LEU A 313 | | 36.976 | 43.031 | 70.903 | 1.00 31.64 | 6 |
| ATOM | 2497 | 0 | LEU A 313 | | 37.605 | 42.793 | 71.925 | 1.00 31.74 | 8 |
| ATCM | 2498 | N | SER A 314 | | 37.206 | 44.064 | 70.099 | 1.00 33.49 | 7 |
| ATOM | 2499 | CA | SER A 314 | | 38.232 | 45.067 | 70.328 | 1.00 35.59 | |
| ATOM | 2500 | CB | SER A 314 | | 38.107 | | | | 6 |
| | 2501 | OG | SER A 314 | | | 46.154 | 69.256 | 1.00 36.47 | 6 |
| ATOM | | | | | 39.141 | 47.120 | 69.353 | 1.00 44.55 | 8 |
| ATCM | 2502 | <u>c</u> | SER A 314 | | 38.046 | 45.661 | 71.730 | 1.30 37.82 | 6 |
| ATOM | 2503 | 0 | SER A 314 | | 39.015 | 46.043 | 72.395 | 1.00 37.32 | 8 |
| ATCM | 2504 | N | GLY A 315 | | 36.794 | 45.725 | 72.175 | 1.00 38.05 | 7 |
| ATOM | 2505 | CA | GLY A 315 | | 36.506 | 46.243 | 73.498 | 1.00 42.42 | 6 |
| ATOM | 2506 | C | GLY A 315 | | 36.295 | 47.744 | 73.568 | 1.00 46.80 | 6 |
| ATOM | 2507 | 0 | GLY A 315 | | 35.923 | 48.276 | 74.618 | 1.00 47.85 | 8 |
| ATCM | 2508 | N | ARG A 316 | | 36.518 | 48.438 | 72.458 | 1.00 48.90 | |
| | | | | | 20.210 | 70.4JO | .4.470 | 7.00 -0.30 | 7. |

| ATOM | | 36.346 | 49.885 | 72.448 | 3 1.00 52.27 | _ |
|--------------|---|------------------|------------------|------------------|--------------------------|--------|
| ATOM | | 37.144 | 50.479 | | | 6 6 |
| ATOM | | 36.730 | 50.007 | | 1.00 52.11 | 6 |
| ATOM | | 37.734 | 50.514 | | 1.00 53.76 | 6 |
| ATOM ATOM | | 39.028 | 49.854 | | 1.00 53.67 | 7 |
| ATOM | 2515 NH1 ARG A 316 | 40.135 | 50.221 | | | 6 |
| MOTA | 2516 NH2 ARG A 316 | 40.110 41.266 | 51.253 | | | 7 |
| ATOM | 2517 C ARG A 316 | 34.882 | 49.546 50.343 | | | 7 |
| ATOM | 2518 O ARG A 316 | 34.075 | 49.781 | | | 6 |
| MOTA | 2519 N GLU A 317 | 34.547 | 51.361 | | | 8 7 |
| MOTA | 2520 CA GLU A.317 | 33.185 | 51.900 | 73.222 | | 6 |
| MOTA . | 2521 CB GLU A 317 | 33.111 | 53.139 | 74.123 | | 6 |
| ATOM | 2522 CG GLU A 317 | 32.549 | 52.901 | 75.527 | | 6 |
| ATOM ATOM | 2523 CD GLU A 317 2524 OE1 GLU A 317 | 33.353 | 51.912 | 76.361 | 1.00 64.62 | 6 |
| ATOM | 2525 OE2 GLU A 317 | 33.025 | 51.741 | 77.556 | | 8 |
| ATOM | 2526 C GLU A 317 | 34.305 32.642 | 51.302 52.256 | 75.832 | | 8 |
| ATOM | 2527 O GLU A 317 | 33.270 | 52.236 | 71.843 71.077 | 1.00 51.27 | 6 |
| MOTA | 2528 N VAL A 318 | 31.457 | 51.733 | 71.548 | 1.00 49.34 1.00 51.30 | 8 7 |
| ATOM | 2529 CA VAL A 318 | | 51.962 | 70.280 | 1.00 48.80 | 6 |
| ATOM | 2530 CB VAL A 318 | 29.522 | 51.071 | 70.169 | 1.00 47.11 | 6 |
| ATOM | 2531 CG1 VAL A 318 | | 51.237 | 68.808 | 1.00 45.53 | 6 |
| ATOM ATOM | 2532 CG2 VAL A 318 2533 C VAL A 318 | | 49.631 | 70.424 | 1.00 47.05 | 6 |
| ATOM | 2534 O VAL A 318 | | 53.411 | 70.178 | 1.00 47.64 | 6 |
| ATOM | 2535 N PRO A 319 | | 53.867 54.165 | 70.953 | 1.00 47.61 | 8 |
| ATOM | 2536 CD PRO A 319 | | 53.836 | 69.234 68.247 | 1.00 48.14 1.00 48.87 | 7 |
| ATOM | 2537 CA PRO A 319 | | 55.569 | 69.093 | 1.00 52.54 | 6 6 |
| ATOM | 2538 CB PRO A 319 | 31.438 | 56.051 | 67.954 | 1.00 49.96 | 6 |
| ATOM | 2539 CG PRO A 319 | | 54.802 | 67.141 | 1.00 50.17 | 6 |
| MOTA MOTA | 2540 C PRO A 319 2541 O PRO A 319 | 29.052 | 55.679 | 68.764 | 1.00 55.84 | 6 |
| ATOM | 2542 N GLU A 320 | | 54.913 | 67.953 | 1.00 56.06 | 8 |
| ATOM | 2543 CA GLU A 320 | | 56.624 56.804 | 69.402 | 1.00 59.20 | 7 |
| ATOM | 2544 CB GLU A 320 | | 57.588 | 69.167 70.313 | 1.00 62.61 | 6 |
| ATOM | 2545 CG GLU A 320 | | 9.042 | 70.365 | 1.00 63.39 | 6 6 |
| ATOM | 2546 CD GLU A 320 | 26.007 5 | 9.823 | 71.451 | 1.00 76.93 | 6 |
| ATOM | 2547 OE1 GLU A 320 | | 9.832 | 71.446 | 1.00 77.37 | 8 |
| ATOM ATOM | 2548 OE2 GLU A 320 2549 C GLU A 320 | | 0.431 | 72.303 | 1.00 79.46 | 8 |
| ATOM | 2549 C GLU A 320 2550 O GLU A 320 | 26.698 5 | 7.551 | 67.863 | 1.00 61.40 | 6 |
| ATOM | 2551 N LYS A 321 | | 8.197 7.463 | 67.699 | 1.00 62.33 | 8 |
| ATOM | 2552 CA LYS A 321 | | 8.150 | 66.939 65.662 | 1.00 59.47 1.00 59.54 | 7 |
| ATOM | 2553 CB LYS A 321 | | 9.648 | 65.897 | 1.00 61.36 | 6 6 |
| ATOM | 2554 CG LYS A 321 | 23.620 6 | 0.323 | 66.366 | 1.00 65.23 | 6 |
| ATOM | 2555 CD LYS A 321 | | 9.691 | 67.643 | 1.00 66.59 | 6 |
| ATOM | 2556 CE LYS A 321 | | 0.215 | 67.960 | 1.00 67.34 | 6 |
| ATOM ATOM | 2557 NZ LYS A 321 2558 C LYS A 321 | | 1.699 | 68.100 | 1.00 68.58 | 7 |
| ATOM | 2559 O LYS A 321 | | | 64.806 | 1.00 59.24 | 6 |
| ATOM | 2560 N LEU A 322 | | | 65.319 63.500 | 1.00 58.70 1.00 57.55 | 8 |
| ATOM | 2561 CA LEU A 322 | | | 62.543 | 1.00 54.72 | 7 6 |
| ATOM | 2562 CB LEU A 322 | | | 61.214 | 1.00 52.96 | 6 |
| MOTA | 2563 CG LEU A 322 | 28.141 5 | 6.316 | 61.295 | 1.00 52.97 | 6 |
| ATOM | 2564 CD1 LEU A 322 | | 5.932 | 59.899 | 1.00 49.01 | 6 |
| MOTA | 2565 CD2 LEU A 322 | | | 62.035 | 1.00 54.73 | 6 |
| ATOM MOTE | 2566 C LEU A 322 2567 O LEU A 322 | | | 62.313 | 1.00 53.47 | .6 |
| MOTA MOTA | 2567 O LEU A 322 2568 N ASN A 323 | | | 62.464 | 1.00 53.39 | 8 |
| ATOM | 2569 CA ASN A 323 | | | | 1.00 51.43 1.00 50.32 | 7 |
| ATOM | 2570 CB ASN A 323 | | | | 1.00 50.32 | 6 6 |
| ATOM | 2571 CG ASN A 323 | - | | | 1.00 55.06 | 6 |
| MOTA | 2572 OD1 ASN A 323 | 34.386 58 | .744 | | 1.00 55.77 | 8 |
| MOTA | 2573 ND2 ASN A 323 | 35.195 60 | .530 | 0.259 | 1.00 52.71 | 7 |
| MOTA | 2574 C ASN A 323 | 31.843 61 | .199 6 | _ | 1.00 48.63 | 6 |
| | | | - | | | |

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| | | | | | • | | | | |
|--------------|---------------|----------|----------------|-------|------------------|------------------|------------------|--------------------------|--------|
| ATOM | | | ASN . | A 323 | 31.13 | 35 60.47 | 9 59.538 | 1.00 47.52 | 2 8 |
| ATOM | | | | A 324 | 32.42 | | 4 59.792 | 1.00 47.66 | |
| ATOM | 257 | | | A 324 | 32.24 | | | | |
| ATOM ATOM | 257 257 | | | A 324 | 32.75 | | | | - |
| ATOM | 258 | | D1 ASN A | | 32.02 | | | | _ |
| ATOM | 258 | | D2 ASN A | | 30.81 32.75 | | | | |
| ATOM | 258 | | ASN A | | 32.90 | | | | |
| ATOM | 258 | | ASN A | | 32.27 | | | | |
| ATOM | 2584 | 1 N | LYS A | | 34.18 | | | | |
| ATOM | 2585 | 5 C | A LYS A | 325 | 34.95 | | | | |
| ATOM | 2586 | | - | | 36.31 | 4 60.45 | 3 57.305 | | |
| MOTA | 2587 | | | | 37.29 | | 7 56.399 | 1.00 54.75 | 6 |
| ATOM | 2588 | | | | 38.56 | | | 1.00 58.22 | |
| ATOM | 2589 2590 | | | | 39.23 | | | 1.00 58.35 | |
| ATOM ATOM | 2591 | | LYS A LYS A | | 40.47 | | | 1.00 59.81 | |
| MOTA | 2592 | | LYS A | | 34.20 34.06 | | | 1.00 44.85 | |
| ATOM | 2593 | | ALA A | | 33.71 | | | 1.00 43.59 1.00 42.27 | |
| ATOM | 2594 | | | | 32.96 | | | 1.00 42.27 | 7 6 |
| ATOM | 2595 | CE | ALA A | 326 | 32.66 | | | 1.00 36.86 | 6 |
| ATOM | 2596 | | ALA A | | 31.66 | | | 1.00 43.30 | |
| MOTA | 2597 | | ALA A | | 31.34 | 2 57.028 | 55.705 | 1.00 42.83 | 8 |
| ATOM | 2598 | | LYS A | | 30.91 | | | 1.00 45.56 | 7 |
| ATOM ATOM | 2599 2600 | | | | 29.65 | | | 1.00 47.23 | 6 |
| ATOM | 2601 | | | | 29.023 28.54 | | | 1.00 49.59 | 6 |
| ATOM | 2602 | CD | | | 28.024 | | | 1.00 54.63 | 6 |
| ATOM | 2603 | CE | | | 27.529 | | | 1.00 55.89 1.00 58.28 | 6 6 |
| MOTA | 2604 | NZ | | | 26.304 | | | 1.00 59.91 | 7 |
| ATOM | 2605 | C | LYS A | | 29.888 | | | 1.00 46.97 | 6 |
| MOTA | 2606 | 0 | LYS A | | 29.090 | | | 1.00 48.10 | 8 |
| ATOM | 2607 | N | GLU A | | | 60.012 | | 1.00 44.99 | 7 |
| MOTA MOTA | 2608 .2609 | CA CB | GLU A | | 31.325 | | | 1.00 43.18 | 6 |
| MOTA | 2610 | CG | GLU A GLU A | | 32.417 31.993 | | | 1.00 47.93 | 6 |
| ATOM | 2611 | CD | GLU A | | 33.112 | | 53.710 53.831 | 1.00 53.65 1.00 55.79 | 6 |
| ATOM | 2612 | | 1 GLU A | | 33.642 | | 52.783 | 1.00 58.73 | 6 8 |
| ATOM | 2613 | | 2 GLU A | | 33.459 | | 54.979 | 1.00 58.13 | 8 |
| ATOM | . 2614 | С | GLU A | 328 | 31.789 | | 52.437 | 1.00 41.56 | 6 |
| ATOM | 2615 | 0 | GLU A | | 31.537 | | 51.255 | 1.00 39.41 | 8 |
| ATOM | 2616 | N | LEU A | | 32.465 | | 53.211 | 1.00 40.64 | 7 |
| ATOM | 2617 2618 | CA | LEU A | | 32.940 | | 52.695 | 1.00 36.45 | 6 |
| ATOM ATOM | 2619 | CB | LEU A | | 33.623 34.100 | | 53.801 | 1.00 34.70 | 6 |
| ATOM | 2620 | | LEU A | | 35.195 | | 53.433 52.359 | 1.00 35.69 | 6 |
| ATOM | 2621 | | LEU A | | 34.619 | | 54.683 | 1.00 30.11 1.00 34.63 | 6 6 |
| ATOM | 2622 | С | LEU A | | 31.746 | | 52.157 | 1.00 35.77 | 6 |
| MOTA | 2623 | 0 | LEU A | 329 | 31.692 | | 50.975 | 1.00 34.94 | 8 |
| ATOM | 2624 | | LEU A | | 30.784 | 55.770 | 53.029 | 1.00 34.78 | 7 |
| ATOM | 2625 | | LEU A | | 29.599 | 55.028 | 52.630 | 1.00 34.95 | 6 |
| ATOM | 2626 | CB | LEU A | | 28.631 | 54.914 | 53.803 | 1.00 30.95 | 6 |
| MOTA | 2627 | CG | LEU A | | 29.164 | 54.115 | 54.991 | 1.00 32.66 | 6 |
| ATOM ATOM | 2628 2629 | | LEU A | | 28.051 29.674 | 53.904 | 56.022 | 1.00 31.74 | 6 |
| ATOM | 2630 | C | LEU A | | 28.877 | 52.769 | 54.509 51.428 | 1.00 30.73 | 6 |
| ATOM | 2631 | ō | LEU A | | 28.395 | 55.631 54.901 | 50.557 | 1.00 37.28 1.00 40.56 | 6 8 |
| ATOM | 2632 | N | LYS A | | 28.806. | 56.957 | 51.383 | 1.00 38.24 | 7 |
| ATOM | 2633 | CA | LYS A | | 28.140 | 57.661 | 50.294 | 1.00 39.59 | 6 |
| ATOM | 2634 | CB | LYS A | | 27.994 | 59.146 | 50.643 | 1.00 42.31 | č |
| ATOM | 2635 | CG | LYS A | | 27.129 | 59.399 | 51.873 | 1.00 45.93 | 6 |
| ATOM | 2636 | CD | LYS A | | 27.017 | 60.879 | 52.244 | 1.00 49.72 | 6 |
| ATOM | 2637 | CE | LYS A | | 26.271 | 61.698 | 51.193 | 1.00 53.66 | 6 |
| ATOM | 2638 | NZ | LYS A 3 | | 26.053 | 63.114 | 51.640 | 1.00 54.22 | 7 |
| ATOM STOM | 2639 2640 | С 0 | LYS A | | 28.863 28.220 | 57.514 | 48.958 | 1.00 41.02 | 6 |
| atom _ | ±04U | 0 | mra w | | 40.440 | 57.485 | 47.904 | 1.00 39.58 | 8 |

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Figure 17-41

| MOTA | 2641 | N SER A 332 | 30.192 | 57.413 | 49.005 | 1.00 42.69 | 7 |
|------|------|---------------|--------|--------|-----------------------|------------|---|
| | 2642 | | | | | | |
| MOTA | | | 30.998 | | | | 6 |
| MOTA | 2643 | CB SER A 332 | 32.494 | 57.243 | 48.124 | 1.00 47.51 | 6 |
| MOTA | 2644 | OG SER A 332 | 32.862 | 56.066 | 48.823 | 1.00 50.97 | 8 |
| ATOM | 2645 | | 30.634 | | 47.040 | 1.00 48.51 | |
| | | | | | | | 6 |
| MOTA | 2646 | | 30.706 | | 45.811 | 1.00 49.45 | 8 |
| MOTA | 2647 | N ILE A 333 | 30.241 | 54.982 | 47.786 | 1.00 51.56 | 7 |
| ATOM | 2648 | CA ILE A 333 | 29.869 | 53.713 | 47.187 | 1.00 54.86 | 6 |
| ATOM | 2649 | CB ILE A.333 | 29.657 | | 48.246 | | |
| | | | | | | | 6 |
| ATOM | 2650 | CG2 ILE A 333 | 29.388 | | 47.559 | 1.00 52.34 | 6 |
| ATOM | 2651 | CG1 ILE A 333 | 30.892 | 52.522 | 49.140 | 1.00 56.89 | 6 |
| MOTA | 2652 | CD1 ILE A 333 | 30.766 | 51.456 | 50.204 | 1.00 60.31 | 6 |
| | 2653 | C ILE A 333 | 28.579 | 53.813 | | | |
| ATOM | | | | | 46.396 | 1.00 57.07 | 6 |
| MOTA | 2654 | O ILE A 333 | 27.572 | 54.321 | 46.897 | 1.00.55.59 | 8 |
| MOTA | 2655 | N ASP A 334 | 28.623 | 53.320 | 45.160 | 1.00 61.14 | 7 |
| MOTA | 2656 | CA ASP A 334 | 27.456 | 53.300 | 44.281 | 1.00 65.55 | 6 |
| | 2657 | CB ASP A 334 | 27.888 | 53.259 | 42.811 | | |
| ATOM | | | | | and the second second | 1.00 69.19 | 6 |
| MOTA | 2658 | CG ASP A 334 | 28.784 | 52.073 | 42.491 | 1.00 70.21 | 6 |
| ATOM | 2659 | OD1 ASP A 334 | 29.097 | 51.875 | 41.298 | 1.00 71.47 | 8 |
| MOTA | 2660 | OD2 ASP A 334 | 29.181 | 51.344 | 43.427 | 1.00 70.91 | 8 |
| | 2661 | C ASP A 334 | 26.660 | 52.041 | 44.627 | | |
| ATOM | | | | | | 1.00 65.65 | 6 |
| MOTA | 2662 | O ASP A 334 | 26.797 | 50.996 | 43.990 | 1.00 63.91 | 8 |
| ATOM | 2663 | N PHE A 335 | 25.822 | 52.153 | 45.649 | 1.00 65.73 | 7 |
| ATOM | 2664 | CA PHE A 335 | 25.041 | 51.021 | 46.104 | 1.00 63.44 | 6 |
| ATOM | 2665 | CB PHE A 335 | 24.980 | 51.034 | 47.632 | 1.00 58.05 | 6 |
| | 2666 | | | | | | |
| MOTA | | | 24.039 | 50.028 | 48.195 | 1.00 53.82 | 6 |
| MOTA | 2667 | CD1 PHE A 335 | 24.178 | 48.679 | 47.886 | 1.00 52.40 | 6 |
| ATOM | 2668 | CD2 PHE A 335 | 22.978 | 50.429 | 48.989 | 1.00 51.33 | 6 |
| ATOM | 2669 | CE1 PHE A 335 | 23.265 | 47.742 | 48.356 | 1.00 52.73 | 6 |
| ATOM | 2670 | CE2 PHE A 335 | 22.062 | 49.503 | 49.462 | 1.00 53.20 | 6 |
| | | | | | | | |
| ATOM | 2671 | CZ PHE A 335 | 22.204 | 48.151 | 49.144 | 1.00 51.76 | 6 |
| MOTA | 2672 | C PHE A 335 | 23.629 | 50.893 | 45.535 | 1.00 65.55 | 6 |
| ATOM | 2673 | O PHE A 335 | 23.230 | 49.810 | 45.097 | 1.00 67.33 | 8 |
| ATOM | 2674 | N GLU A 336 | 22.874 | 51.986 | 45.537 | 1.00 66.47 | 7 |
| | 2675 | CA GLU A 336 | 21.497 | 51.948 | | | 6 |
| ATOM | | | | | 45.048 | 1.00 67.43 | |
| ATOM | 2676 | CB GLU A 336 | 21.422 | 51.379 | 43.626 | 1.00 71.79 | 6 |
| ATOM | 2677 | CG GLU A 336 | 19.982 | 51.245 | 43.116 | 1.00 78.77 | 6 |
| ATOM | 2678 | CD GLU A 336 | 19.868 | 50.505 | 41.789 | 1.00 82.67 | 6 |
| MOTA | 2679 | OE1 GLU A 336 | 20.232 | 49.306 | 41.734 | 1.00 83.29 | 8 |
| | 2680 | | | | | | |
| ATOM | | | 19.410 | 51.126 | 40.801 | 1.00 84.26 | 8 |
| ATOM | 2681 | C GLU A 336 | 20.655 | 51.069 | 45.971 | 1.00 64.72 | 6 |
| ATOM | 2682 | O GLU A 336 | 20.686 | 49.840 | 45.876 | 1.00 59.84 | 8 |
| ATOM | 2683 | N GLU A 337 | 19.901 | 51.710 | 46.858 | 1.00 64.47 | 7 |
| ATOM | 2684 | CA GLU A 337 | 19.045 | 51.003 | 47.805 | 1.00 65.83 | 6 |
| | 2685 | | | | | | |
| ATOM | | CB GLU A 337 | 18.398 | 52.003 | 48.759 | 1.00 64.20 | 6 |
| MOTA | 2686 | CG GLU A 337 | 17.753 | 51.3~0 | 49.964 | 1.00 64.26 | 6 |
| ATOM | 2687 | CD GLU A 337 | 18.774 | 0ز€.50 | 50.850 | 1.00 64.04 | 6 |
| ATOM | 2688 | OE1 GLU A 337 | 19.741 | 51.3.2 | 51.261 | 1.00 61.66 | 8 |
| | 2689 | OE2 GLU A 337 | 18.608 | 49.483 | 51.132 | 1.00 63.64 | 8 |
| MOTA | | | | | | | |
| ATOM | 2690 | C GLU A 337 | 17.950 | 50.239 | 47.063 | 1.00 67.13 | 6 |
| ATOM | 2691 | O GLU A 337 | 17.269 | 50.807 | 46.205 | 1.00 68.27 | 8 |
| ATOM | 2692 | N PHE A 338 | 17.779 | 48.960 | 47.394 | 1.00 67.22 | 7 |
| ATOM | 2693 | CA PHE A 338 | 16.764 | 48.129 | 46.748 | 1.00 68.05 | 6 |
| | | | | | | | |
| ATOM | 2694 | CB PHE A 338 | 16.445 | 46.919 | 47.626 | 1.00 69.68 | 6 |
| MOTA | 2695 | CG PHE A 338 | 15.228 | 46.158 | 47.187 | 1.00 72.35 | 6 |
| ATOM | 2696 | CD1 PHE A 338 | 15.122 | 45.674 | 45.888 | 1.00 72.37 | 6 |
| ATOM | 2697 | CD2 PHE A 338 | 14.172 | 45.941 | 48.074 | 1.00 73.61 | 6 |
| | • | | | | | | |
| ATOM | 2698 | CE1 PHE A 338 | 13.980 | 44.984 | 45.478 | 1.00 73.39 | 6 |
| ATOM | 2699 | CE2 PHE A 338 | 13.024 | 45.250 | 47.672 | 1.00 73.26 | 6 |
| ATOM | 2700 | CZ PHE A 338 | 12.929 | 44.771 | 46.369 | 1.00 73.34 | 6 |
| ATOM | 2701 | C PHE A 338 | 15.481 | 48.902 | 46.434 | 1.00 68.45 | 6 |
| | 2702 | | 15.286 | 49.367 | | 1.00 67.92 | 8 |
| MOTA | | O PHE A 338 | | | 45.310 | | |
| ATOM | 2703 | N ASP A 339 | 14.606 | 49.026 | 47.426 | 1.00 68.98 | 7 |
| ATOM | 2704 | CA ASP A 339 | 13.358 | 49.759 | 47.261 | 1.00 70.68 | 6 |
| ATOM | 2705 | CB ASP A 339 | 12.596 | 49.758 | 48.588 | 1.00 71.06 | 6 |
| - | 2706 | CG ASP A 339 | 11.381 | 50.678 | 48.581 | 1.00 72.05 | 6 |
| MOTA | 2,00 | CG ROP N 333 | | -0.070 | - 30.10T | 1.00 /2.00 | ٠ |
| | | | | | | | |

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| MOTA | 2707 | OD | 1 ASP A 339 | | 11.548 | 51.893 | 48.320 | 1.00 72.29 | 8 |
|--------------|--------------|----------|----------------------------|---|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 2708 | OD | 2'ASP A 339 | | 10.262 | 50.188 | 48.858 | | 8 |
| ATOM | 2709 | С | ASP A 339 | | 13.715 | 51.183 | 46.853 | 1.00 73.18 | 6 |
| ATOM | 2710 | 0 | ASP A 339 | | 14.407 | | 47.592 | 1.00 73.78 | 8 |
| ATOM | 2711 | N | ASP A 340 | | 13.247 | 51.600 | 45.677 | 1.00 76.36 | 7 |
| ATOM | 2712 | CA | ASP A 340 | | 13.518 | 52.943 | 45.152 | 1.00 78.34 | 6 |
| MOTA | 2713 | CB | _ASP A 340 | | 12.410 | 53.385 | 44.189 | 1.00 77.55 | 6 |
| MOTA | 2714 | | | • | 12.462 | 52.655 | 42.864 | 1.00 78.90 | 6 |
| ATOM | 2715 | | 1 ASP A 340 | | 12.348 | 51.408 | 42.855 | 1.00 78.38 | 8 |
| MOTA | 2716 | | 2 ASP A 340 | | 12.620 | 53.336 | 41.830 | 1.00 78.74 | 8 |
| ATOM | 2717 | | ASP A 340 | - | 13.687 | 54.017 | 46.214 | 1.00 79.51 | 6 |
| MOTA | 2718 | | ASP A 340 | | 14.587 | 54.856 | 46.117 | 1.00 80.19 | 8 |
| ATOM | 2719 | N | GLU A 341 | | 12.824 | 54.000 | 47.224 | 1.00 79.64 | 7 |
| ATOM | 2720 | | GLU A 341 | | 12.922 | 54.998 | 48.271 | 1.00 80.05 | 6 |
| ATOM | 2721 | CB | GLU A 341 | | 12.269 | 56.301 | 47.811 | 1.00 83.75 | 6 |
| ATOM | 2722 | CG | GLU A 341 | | 12.411 | 57.442 | 48.806 | 1.00 89.02 | 6 |
| ATOM | 2723 | | GLU A 341 | | 11.756 | 58.724 | 48.328 | 1.00 91.52 | 6 |
| ATOM | 2724 2725 | OE. | 1 GLU A 341 2 GLU A 341 | | 10.515 | 58.738 | 48.175 | 1.00 93.33 | 8 |
| MOTA | 2726 | C | GLU A 341 | | 12.484 | 59.716 | 48.102 | 1.00 92.65 | 8 |
| MOTA | 2727 | o | GLU A 341 | | 12.317 11.102 | 54.578 54.610 | 49.597 49.777 | 1.00 77.98 | 6 |
| ATOM ATOM | 2728 | N | VAL A 342 | | 13.179 | 54.181 | 50.523 | 1.00 79.82 1.00 74.49 | 8 |
| ATOM | 2729 | CA | VAL A 342 | • | 12.745 | 53.793 | 51.859 | 1.00 74.49 | 7 6 |
| ATOM | 2730 | СВ | VAL A 342 | | 13.224 | 52.383 | 52.245 | 1.00 71.33 | 6 |
| ATOM | 2731 | | L VAL A 342 | | 12.672 | 52.004 | 53.610 | 1.00 72.40 | 6 |
| ATOM | 2732 | | VAL A 342 | | 12.797 | 51.391 | 51.207 | 1.00 74.35 | 6 |
| ATOM | 2733 | С | VAL A 342 | | 13.454 | 54.778 | 52.766 | 1.00 68.46 | 6 |
| ATOM | 2734 | 0 | VAL A 342 | | 12.952 | 55.154 | 53.829 | 1.00 68.96 | 8 |
| ATOM | 2735 | N | ASP A 343 | | 14.636 | 55.184 | 52.311 | 1.00 61.61 | 7 |
| A'TOM | 2736 | CA | ASP A 343 | | 15.486 | 56.114 | 53.029 | 1.00 54.91 | 6 |
| MOTA | 2737 | CB | ASP A 343 | | 14.678 | 57.303 | 53.543 | 1.00 55.06 | 6 |
| MOTA | 2738 | CG | ASP A 343 | | 15.556 | 58.390 | 54.114 | 1.00 54.44 | 6 |
| ATOM | 2739 | | ASP A 343 | | 15.002 | 59.351 | 54.694 | 1.00 56.20 | 8 |
| ATOM | 2740 | - | ASP A 343 | • | 16.795 | 58.287 | 53.969 | 1.00 49.32 | 8 |
| MOTA | 2741 | C | ASP A 343 | | 16.152 | 55.401 | 54.198 | 1.00 50.85 | 6 |
| MOTA | 2742 | O N | ASP A 343 | | 15.557 | 55.209 | 55.257 | 1.00 49.32 | 8 |
| MOTA | 2743 2744 | N CA | ARG A 344 ARG A 344 | | 17.396 18.195 | 55.004 54.321 | 53.980 | 1.00 47.84 | 7 |
| ATOM ATOM | 2745 | CB | ARG A 344 | | 18.883 | 53.099 | 54.981 54.358 | 1.00 45.34 1.00 45.00 | 6 6 |
| ATOM | 2746 | CG | ARG A 344 | | 17.950 | 51.969 | 53.974 | 1.00 38.03 | 6 |
| ATOM | 2747 | CD | ARG A 344 | | 17.185 | 51.531 | 55.188 | 1.00 35.83 | 6 |
| ATOM | 2748 | NE | ARG A 344 | | 16.278 | 50.439 | 54.885 | 1.00 39.20 | 7 |
| ATOM | 2749 | CZ | ARG A 344 | | 15.350 | 49.993 | 55.724 | 1.00 39.89 | 6 |
| ATOM | 2750 | NH1 | ARG A 344 | | 15.217 | 50.561 | 56.917 | 1.00 40.17 | 7 |
| ATOM | 2751 | NH2 | ARG A 344 | | 14.566 | 48.976 | 55.375 | 1.00 40.75 | 7 |
| ATC I | 2752 | С | ARG A 344 | | 19.250 | 55.278 | 55.515 | 1.00 44.72 | 6 |
| ATC:M | 2753 | 0 | ARG A 344 | | 20.170 | 54.869 | 56.223 | 1.00 46.97 | 8 |
| atom | 2754 | N | SER A 345 | | 19.113 | 56.552 | 55.157 | 1.00 45.81 | 7. |
| ATOM | 2755 | CA | SER A 345 | | 20.045 | 57.596 | 55.577 | 1.00 43.66 | 6 |
| MOTA | 2756 | CB | SER A 345 | | 19.538 | 58.960 | 55.115 | 1.00 43.44 | 6 |
| ATOM | 2757 | OG | SER A 345 | | 18.292 | 59.260 | 55.722 | 1.00 45.62 | 8 |
| ATOM | 2758 | C | SER A 345 | | 20.258 | 57.627 | 57.089 | 1.00 42.79 | 6 |
| ATOM | 2759 | 0 | SER A 345 | | 21.364 | 57.902 | | 1.00 42.62 | 8 |
| ATOM | 2760 | N | TYR A 346 | | 19.200 | 57.354 | 57.851 | 1.00 40.55 | 7 |
| ATOM | 2761 | CA CB | TYR A 346 TYR A 346 | | 19.280 | 57.352 | 59.308 | 1.00 41.05 | 6 |
| ATOM | 2762 | CG | TYR A 346 | | 17.971 | 56.819 | 59.905 | 1.00 41.74 | 6 |
| ATOM | 2763 2764 | CD1 | TYR A 346 | | 17.668 18.331 | 55.355 54 333 | 59.630 60.328 | 1.00 43.47 | 6 |
| ATOM | 2764 2765 | | TYR A 346 | | 18.044 | 54.333 52.983 | 60.328 | 1.00 44.45 1.00 41.02 | 6 6 |
| ATOM | 2766 | | TYR A 346 | | 16.710 | 54.988 | 58.682 | 1.00 41.02 | 6 |
| ATOM ATOM | 2767 | CE2 | TYR A 346 | | 16.710 | 53.644 | 58.434 | 1.00 42.08 | 6 |
| aton atom | 2768 | CZ | TYR A 346 | | 17.086 | 52.649 | 59.139 | 1.00 41.66 | 5 |
| ATCM | 2769 | ОН | TYR A 346 | | 16.806 | 51.324 | 58.884 | 1.00 39.60 | 8 |
| ATCM | 2770 | C | TYR A 346 | | 20.466 | .56.517 | 59.796 | 1.00 42.92 | 6 |
| ATCM | 2771 | ō | TYR A 346 | | 21.101 | 56.844 | 60.799 | 1.00 42.65 | 8 |
| ATCM ATCM | 2772 | N | MET A 347 | | 20.757 | 55.443 | 59.067 | 1.00 44.59 | 7 |
| | | | | | | | _ | | |

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Figure 17-43

| ATOM | 2773 | CA MET A 3 | 47 21.859 | 54.546 | 59.388 | 1.00 45,89 | 6 |
|--------|--------|--------------|------------------------|----------------|----------------|--------------|-----|
| | | | | | | | |
| ATOM | 2774 | | | | 58.353 | 1.00 45.51 | 6 |
| ATOM | . 2775 | CG MET A 3 | 47 20.727 | 52.567 | 58.244 | 1.00 45.01 | 6 |
| ATOM | 277€ | SD MET A 3 | 47 21.062 | 51.258 | 57.066 | 1.00 47.13 | 16 |
| | | | | | | | |
| ATOM | 2777 | | | | 55.676 | 1.00 44.55 | 6 |
| ATOM - | 2778 | C MET A 3 | | | 59.404 | 1.00 48.47 | 6 |
| MOTA | 2779 | O MET A 3 | 47 24.129 | 54.888 | 60.098 | 1.00 49.49 | 8 |
| | 2780 | | | | 58.610 | 1.00 49.03 | |
| MOTA | | | | | | | 7 |
| MOTA | 2781 | CA LEUA 3 | 48 24.458 | 57.178 | 58.499 | 1.00 48.86 | 6 |
| MOTA | 2782 | CB LEU A 3 | 48 24.355 | 58.082 | 57.269 | 1.00 45.51 | 6 |
| | 2783 | | | | 55.895 | 1.00 44.47 | |
| ATOM | | | | | | | 6 |
| ATOM | 2784 | | | | 54.859 | 1.00 43.62 | 6 |
| ATOM | 2785 | CD2 LEU A 3 | 48 ⁻ 25.618 | 56.757 | 55.565 | - 1.00 42.53 | 6 |
| ATOM | 2786 | C LEU A 3 | 48 24.644 | 58.049 | 59.738 | 1.00 49.33 | 6 |
| | | | | | | | |
| ATOM | 2787 | | | | 60.123 | 1.00 49.78 | 8 |
| MOTA | 2788 | N GLU A 3 | 49 23.537 | 58.428 | 60.358 | 1.00 48.34 | 7. |
| MOTA | 2789 | CA GLU A 3 | 49 23.591 | 59.279 | 61.533 | 1.00 49.24 | 6 |
| | 2790 | | | 59.848 | 61.811 | 1.00 48.36 | 6 |
| MOTA | | | | | | | |
| MOTA | 2791 | CG GLU A 3 | | 60.584 | 60.607 | 1.00 45.52 | 6 |
| ATOM | 2792 | CD GLU A 3 | 49 22.598 | 61.619 | 60.065 | 1.00 42.94 | 6 |
| ATOM | 2793 | OE1 GLU A 3 | 19 22.934 | 62.560 | 60.812 | 1.00 40.82 | 8 |
| | 2794 | OE2 GLU A 3 | | | | | |
| ATOM | | | | 61.483 | 58.900 | 1.00 38.30 | 8 |
| ATOM | 2795 | C GLU A 3 | | 58.531 | 62.745 | 1.00 48.32 | 6 |
| ATOM | 2796 | O GLU A 3 | 19 25.226 | 58.783 | 63.219 | 1.00 47.87 | 8 |
| | 2797 | N THR A 3 | | 57.602 | 63.248 | 1.00 48.97 | 7 |
| ATOM | | | | | | | |
| ATOM | 2798 | CA THR A 3 | | 56.832 | 64.398 | 1.00 50.70 | 6 |
| ATOM | 2799 | CB THR A 3 | 50 22.558 | 56.596 | 65.342 | 1.00 51.02 | 6 |
| ATOM | 2800 | OG1 THR A 35 | 50 22.071 | 57.865 | 65.803 | 1.00 49.11 | 8 |
| ATOM | 2801 | CG2 THR A 35 | 50 22.983 | 55.763 | 66.537 | 1.00 51.58 | 6 |
| | 2802 | C THR A 3 | | 55.507 | 63.954 | 1.00 49.56 | |
| MOTA | | | | | | | 6 |
| MOTA | 2803 | O THR A 35 | 23.979 | 54.947 | 62.923 | 1.00 50.55 | 8 |
| ATOM | 2804 | N LEU A 35 | 51 25.333 | 55.028 | 64.725 | 1.00 46.88 | 7 |
| ATOM | 2805 | CA LEU A 35 | 26.018 | 53.781 | 64.417 | 1.00 45.35 | 6 |
| | 2806 | CB LEU A 35 | | 53.726 | 65.185 | 1.00 47.05 | 6 |
| MOTA | | | | | | | |
| MOTA | 2807 | CG LEU A 35 | | 52.502 | 65.072 | 1.00 49.54 | 6 |
| ATOM | 2808 | CD1 LEU A 35 | 29.575 | 52 <i>.777</i> | 65.766 | 1.00 51.50 | 6 |
| MOTA | 2809 | CD2 LEU A 35 | 27.603 | 51.302 | 65.692 | 1.00 48.35 | 6 |
| | 2810 | C LEU A 35 | | 52.584 | 64.772 | 1.00 44.79 | 6 |
| ATOM | | | | | | | |
| MOTA | 2811 | O LEU A 35 | | 51.578 | 64.061 | 1.00 41.45 | 8 |
| ATOM . | 2812 | N LYS A 35 | 24.420 | 52.711 | 65.880 | 1.00 45.27 | 7 |
| ATOM | 2813 | CA LYS A 35 | 2 23.531 | 51.662 | 66.375 | 1.00 44.62 | 6 |
| | 2814 | CB LYS A 35 | | 51.464 | 67.873 | 1.00 42.23 | 6 |
| ATOM | | | | | | | |
| ATOM | 2815 | CG LYS A 35 | | 51.075 | 68.187 | 1.00 44.94 | 6 |
| ATOM | 2816 | CD LYS A 35 | 2 25.572 | 51.262 | 69 .650 | 1.00 46.80 | 6 |
| ATOM | 2817 | CE LYS A 35 | 2 24.765 | 50.389 | 70.581 | 1.00 45.79 | 6 |
| | 2818 | NZ LYS A 35 | 2 25.236 | 50.586 | 71.975 | 1.00 47.31 | 7 |
| ATOM | | | | | | 1.00 45.12 | 6 |
| ATOM | 2819 | | | 52.087 | 66.116 | | |
| MOTA | 2820 | O LYS A 35 | | 53.236 | 65. 756 | 1.00 47.07 | 8 |
| ATOM | 2821 | N ASP A 35 | 3 21.162 | 51.161 | 66.285 | 1.00 44.62 | 7 · |
| ATOM | 2822 | CA ASP A 35 | 3 19.761 | 51.474 | 66.060 | 1.00 46.43 | 6 |
| | | | | 50.943 | | | |
| MOTA | 2823 | CB ASP A 35 | | | 64.692 | 1.00 49.38 | 6 |
| MOTA | 2824 | | | 49.546 | 64.396 | .1.00 51.52 | 6 |
| ATOM | 2825 | OD1 ASP A 35 | 3 21.028 | 49.396 | 64.158 | 1.00 55.36 | 8 |
| | 2826 | OD2 ASP A 35 | | 48.596 | 64.398 | 1.00 52.35 | 8 |
| ATOM | | | · | | | | |
| MOTA | 2827 | C ASP A 35 | | 50.968 | 67.165 | 1.00 45.90 | 6 |
| ATOM | 2828 | O ASP A 35 | | 50.001 | 67.854 | 1.00 45.98 | 8 |
| ATOM | 2829 | N PRO A 35 | 4 17.687 | 51.629 | 67.348 | 1.00 45.86 | 7 |
| | 2830 | CD PRO A 35 | | 52.775 | 66.587 | 1.00 45.36 | 6 |
| ATOM | | | | | | | |
| MOTA | 2831 | CA PRO A 35 | | 51.243 | 68.378 | 1.00 45.52 | 6 |
| ATOM | 2832 | CB PRO A 35 | 4 15.585 | 52.245 | 68 .159 | 1.00 44.77 | 6 |
| MOTA | 2833 | CG PRO A 35 | 4 15.681 | 52.513 | 66.664 | 1.00 45.06 | 6 |
| | 2834 | C PRO A 35 | | 49.804 | 68.188 | 1.00 44.13 | 6 |
| ATOM | | | | | _ | | |
| ATOM | 2835 | O PRO A 35 | | 49.271 | 67.078 | 1.00 42.90 | 8 |
| ATCM | 2836 | N TRP A 35 | 5 15.821 | 49.174 | 69. 267 | 1.00 42.77 | 7 |
| ATOM | 2837 | CA TRP A 35 | 5 15.358 | 47.801 | 69.168 | 1.00 43.35 | 6 |
| | 2838 | CB TRP A 35 | | 47.225 | 70.539 | 1.00 47.11 | 6 |
| ATOM | 2000 | | | - 1 . 22 - | | | - |

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| ATO: | M 2839 CG TRP A 355 | 16.168 46.752 71.322 1.00 52 43 |
|--------------|--|--|
| ATO | M 2840 CD2 TRP A 355 | 16 574 45 391 71 510 1 00 52.43 |
| OTA OTA | 11 333 | 17.789 45.416 72.238 1.00 54 97 6 |
| ATO | | 16.031 44.153 71.155 1.00 53 39 6 |
| ATO | 31 333 | 17.125 47.526 71.916 1.00 54.39 6 |
| ATO | 21 333 | 18.103 46.731 72.468 1.00 57.31 7 |
| ATON | | 18.469 44.249 72.602 1.00 54.97 6 16.706 42.995 71.518 1.00 55.77 |
| 1OTA | 4 2847 CH2 TRP A 355 | |
| ATON | 1 2848 C TRP A 355 | 14 177 47 600 60 220 2 00 14.04 6 |
| MOTA | 4 2849 O TRP A 355 | 13 508 49 677 67 015 4 00 41.94 6 |
| ATOM | | 13 942 46 471 67 775 1 20 21.39 8 |
| ATOM | | 12.855 46.185 66.866 1.00 36.55 6 |
| ATOM ATOM | | 13.413 46.044 65.451 1.00 35.06 6 |
| ATOM | | 14.120 47.308 64.976 1.00 32.47 6 |
| ATOM | | 14.969 47.082 63.733 1.00 29.54 6 |
| ATOM | 110 11 330 | 15.600 48.323 63.296 1.00 28.91 7 |
| ATOM | | 16.514 48.403 62.335 1.00 30.60 6 16.916 47.305 61.702 1.00 33.53 |
| ATOM | 2858 NH2 ARG A 356 | 1.00 33.32. |
| ATOM | 2859 C ARG A 356 | 10 30.10 |
| ATOM | 2860 O ARG A 356 | 12 447 43 931 66 742 1 00 36.01 6 |
| MOTA | | 11.587 44.949 68.499 1.00 36.04 7 |
| MOTA MOTA | 00.40 | 11.001 43.758 69.085 1.00 36.08 6 |
| MOTA | 2863 C GLY A 357 2864 O GLY A 357 | 9.514 43.596 68.851 1.00 34.51 6 |
| ATOM | 2864 O GLY A 357 2865 N GLY A 358 | 8.943 44.196 67.943 1.00 36.77 8 |
| ATOM | 2866 CA GLY A 358 | 8.892 42.772 69.687 1.00 36.04 7 |
| ATOM | 2867 C GLY A 358 | 7.466 42.506 69.593 1.00 32.26 6 7.106 41.263 70 385 1.00 32.26 6 |
| ATOM | 2868 O GLY A 358 | 1.00 23.03 6 |
| MOTA | 2869 N GLU A 359 | 200 20.00 8 |
| ATOM | 2870 CA GLU A 359 | 5 550 39 455 70 742 7 00 30.08 / |
| ATOM | 2871 CB GLU A 359 | 4.034 39.289 70.604 1.00 32.58 6 |
| ATOM ATOM | 2872 CG GLU A 359 2873 CD GLU A 359 | 3.230 40.435 71.222 1.00 47.44 6 |
| ATOM | 2873 CD GLU A 359 2874 OE1 GLU A 359 | 1.957 40.762 70.445 1.00 50.93 6 |
| ATOM | 2875 OE2 GLU A 359 | 1.123 39.852 70.221 1.00 52.13 8 1.798 41.942 70.061 1.00 51.03 |
| ATOM | 2876 C GLU A 359 | 6.250 39.275 70.000 |
| MOTA | 2877 O GLU A 359 | 6 790 38 383 68 003 1 00 20.23 |
| ATOM | 2878 N VAL A 360 | 6 263 37 147 70 700 |
| ATOM | 2879 CA VAL A 360 | 6.859 35.957 70.193 1.00 25.86 6 |
| ATOM ATOM | 2880 CB VAL A 360 2881 CG1 VAL A 360 | 7.6/3 35.168 71.237 1.00 22.02 6 |
| ATOM | 2881 CG1 VAL A 360 2882 CG2 VAL A 360 | 8.155 33.849 70.641 1.00 19.45 6 |
| ATOM | 2883 C VAL A 360 | 8.850 36.009 71.698 1.00 17.88 6 |
| ATOM | 2884 C VAL A 360 | 4 942 34 655 80 413 |
| ATOM | 2885 N ARG A 361 | 5 663 34 000 60 350 1 30 27.34 8 |
| - MOTA | 2886 C., ARG A 361 | 4 612 34 001 67 767 |
| MOTA | 2887 CB ARG A 361 | 4.693 34.164 66.242 1.00 32.85 6 |
| MOTA | 2888 CG ARG A 361 | 4.243 35.504 65.687 1.00 38.81 6 |
| MOTA MOTA | 2889 CD ARG A 361 2890 NE ARG A 361 | 4.546 35.653 64.201 1.00 40.09 6 |
| ATOM | 2890 NE ARG A 361 2891 CZ ARG A 361 | 5.9/4 35.812 63.961 1.00 38.77 7 |
| ATOM | 2892 NH1 ARG A 361 | 6.514 35.989 62.763 1.00 39.21 6 5.748 36.027 61.685 1.00 40.78 |
| ATOM | 2893 NH2 ARG A 361 | 7 822 36 145 62 642 1 00 10.75 |
| ATOM | 2894 C ARG A 361 | 4 689 32 628 68 323 |
| MOTA | 2895 O ARG A 361 | 5 769 33 007 68 471 |
| MOTA | 2896 N LYS A 362 | 3.526 32.017 68.347 1.00 37.08 8 |
| MOTA | 2897 CA LYS A 362 | 3.436 30.626 68.757 1.00 39.91 6 |
| ATOM | 2898 CB LYS A 362 2899 CG LYS A 362 | 1.982 30.152 68.648 1.00 43.43 6 |
| MOTA MOTA | 2899 CG LYS A 362 2900 CD LYS A 362 | 1.014 30.803 69.640 1.00 45.11 6 |
| ATOM | 2900 CD LYS A 362 2901 CE LYS A 362 | 1.117 32.346 69.673 1.00 49.43 6 |
| TOM | 2902 NZ LYS A 362 | 0.813 33.022 68.327 1.00 45.02 6 |
| TOM | 2903 C LYS A 362 | 4 320 20 000 67 021 |
| MOTA | 2904 O LYS A 362 | 4 953 38 035 69 340 1 00 35.23 |
| | • | 4.223 20.835 08.248 1.UU 35.45 g |

| | • | | | | |
|---------------------------|-------------------|-----------|-----------|-------------|-----|
| ATOM 2905 N GLU A | 363 4 3 | | | | |
| | | | | | 3 7 |
| | | | 65.539 | 1.00 43.9 | 5 6 |
| ATOM 2907 CB GLU A | | 25 30.416 | 64.278 | | , , |
| ATOM 2908 CG GLU A | 363 3.89 | | | | 9 6 |
| ATOM 2909 CD GLU A | 2 6 2 | | 63.741 | | 36 |
| ATOM 2910 OE1 GLU A | | | 62.507 | 1.00 54.11 | 6 ا |
| | | 71 31.224 | 61.494 | 1.00 53.90 | 1 0 |
| ATOM 2911 OE2 GLU A | 363 3 <i>.</i> 64 | 8 32.927 | 62.552 | 1 00 55 55 | 8 |
| ATOM 2912 C GLU A | 363 6.55 | 8 29.296 | 66 046 | 1.00 56.05 | 8 |
| ATOM 2913 O GLU A | | 23.230 | 66.046 | 1.00 42.39 | 6 |
| | | | 65.989 | 1.00 41.48 | 8 |
| | | 3 30.360 | 66.540 | 1.00 37.27 | 7 |
| ATOM 2915 CA VAL A | 364 8.53 | 5 30.291 | 67.064 | 2.00 37.27 | |
| ATOM 2916 CB VAL A | | | | 1.00 35.30 | 6 |
| ATOM 2917 CG1 VAL A | | | 67.469 | 1.00 36.88 | 6 |
| AMON 2010 CG1 VAL A | | | 68.043 | 1.00 37.77 | 6 |
| ATOM 2918 CG2 VAL A | | 8 32.628 | 66.252 | 1.00 34.78 | - |
| ATOM 2919 C VAL A: | 164 8.65 | | 68.268 | 1.00 34.78 | |
| ATOM 2920 O VAL A | | | | 1.00 33.01 | 6 |
| 222 | | | 68.379 | 1.00 31.55 | 8 |
| | | | 69.165 | 1.00 32.61 | 7 |
| ATOM 2922 CA LYS A 3 | | 4 28.567 | 70.362 | 1.00 30.96 | |
| ATOM 2923 CB LYS A 3 | 6.59 | 8 29.010 | | 1.00 30.96 | 6 |
| ATOM 2924 CG LYS A 3 | | | 71.358 | 1.00 30.13 | 6 |
| | | 30.409 | 71.899 | 1.00 36.02 | 6 |
| | 65 5.83° | 7 30.781 | 72.995 | 1.00 38.94 | 6 |
| ATOM 2926 CE LYS A 3 | 65 6.120 | 32.187 | 73.509 | 1.00 41.58 | |
| ATOM 2927 NZ LYS A 3 | 65 5.191 | | | 1.00 41.58 | 6 |
| ATOM 2928 C LYS A 3 | | | 74.585 | 1.00 44.29 | 7 |
| ATOM 2929 O LYS A 3 | | | 70.007 | 1.00 30.32 | 6 |
| 5 | | | 70.442 | 1.00 31.32 | 8 |
| ATOM 2930 N ASP A 3 | | 26.863 | 69.209 | 1.00 29.85 | |
| ATOM 2931 CA ASP A 3 | 66 6.115 | | 68.807 | 1.00 29.85 | 7 |
| ATOM 2932 CB ASP A 3 | | | | 1.00 32.07 | 6 |
| ATOM 2933 CG ASP A 3 | 56 3.740 | | 67.818 | 1.00 35.98 | 6 |
| 300M 3034 001 300 5 | | | 68.381 | 1.00 39.88 | 6 |
| ATOM 2934 OD1 ASP A 3 | 56 3.124 | 25.692 | 69.359 | 1.00 40.16 | |
| ATOM 2935 OD2 ASP A 3 | 56 3.326 | | 67.848 | 1 00 40 55 | 8 |
| ATOM 2936 C ASP A 30 | 66 7.343 | | | 1.00 43.21 | 8 |
| ATOM 2937 O ASP A 30 | | | 68.161 | 1.00 33.07 | 6 |
| ATOM 2938 N THR A 36 | _ | 23.763 | 68.540 | 1.00 32.64 | 8 |
| | | 25.565 | 67.193 | 1.00 31.89 | 7 |
| ATOM 2939 CA THR A 36 | 7 9.088 | 25.045 | 66.490 | | |
| ATOM 2940 CB THR A 36 | 7 9.712 | | | 1.00 31.17 | 6 |
| ATOM 2941 OG1 THR A 36 | | | | 1.00 31.55 | 6 |
| ATOM 2942 CG2 THR A 36 | 7 8.707 | | 64.714 | 1.00 34.37 | 8 |
| | | 25.404 | 64.723 | 1.00 33.55 | 6 |
| ATOM 2943 C THR A 36 | 7 10.146 | 24.633 | 67.472 | 1.00 33.09 | |
| ATOM 2944 O THR A 36 | 7 10.586 | | | | 6 |
| ATOM 2945 N LEU A 36 | | | | 1.00 38.62 | 8 |
| ATOM 2946 CA LEU A 36 | | | 68.298 | 1.00 31.85 | 7 |
| | _ | | 69.288 | 1.00 32.87 | 6 |
| ATOM 2947 CB LEU A 36 | 8 11.848 | 26.478 | 70.179 | 1.00 27.73 | 6 |
| ATOM 2948 CG LEU A 36 | 12.887 | | | | |
| ATOM 2949 CD1 LEU A 36 | 3 14.260 | | | 1.00 29.05 | 6 |
| ATOM 2950 CD2 LEU A 36 | | | | 1.00 23.05 | 6 |
| ATOM 2951 C LEU A 36 | | | | 1.00 26.53 | 6 |
| | | 24.053 | 70.107 | 1.00 35.16- | 6 |
| ATOM 2952 O LEU A 368 | 11.910 | | 70.217 | 1.00 35.18 | |
| ATOM 2953 N GLU A 369 | 9.942 | | | | 8 |
| ATOM 2954 CA GLU A 369 | | | | 1.00 37.56 | 7 |
| | | | 71.442 1 | 1.00 40.23 | 6 |
| | ,,,,,, | 23.216 7 | | 1.00 42.07 | 6 |
| ATOM 2956 CG GLU A 369 | | | | 1.00 48.51 | 6 |
| ATOM 2957 CD GLU A 369 | 6.281 | | | | |
| ATOM 2958 OE1 GLU A 369 | | | | .00 51.93 | 6 |
| · ATOM 2959 OE2 GLU A 369 | | | 3.782 1 | 00 52.84 | 8 |
| | | 25.636 7 | 2.710 1 | .00 58.33 | 8 |
| ATOM 2960 C GLU A 369 | 9.633 | | | .00 41.14 | 6 |
| ATOM 2961 O GLU A 369 | 10.087 | | | .00 41.87 | |
| ATOM 2962 N LYS A 370 | 9.309 | | | | 8 |
| | | | 9.411 1 | .00 39.65 | 7 |
| | 9.497 | | 8.636 1 | .00 38.26 | 6 |
| ATOM 2964 CB LYS A 370 | 9.144 | | | .00 40.63 | 6 |
| ATOM 2965 CG LYS A 370 | 7.675 | | 6.854 1 | .00 44.49 | |
| ATOM 2966 CD LYS A 370 | 7.495 | | 5 3 C 3 . | 30 40 - | 6 |
| | | | 5.363 1 | .00 49.95 | 6 |
| | 6.052 | 20.023 6 | 5.015 1. | .00 54.28 | 6 |
| ATOM 2968 NZ LYS A 370 | 5.890 | | 3.574 1. | .00 55.44 | 7 |
| ATOM 2969 C LYS A 370 | 10.948 | | 3.730 1. | .00 37.85 | |
| ATOM 2970 O LYS A 370 | 11.261 | |) 150 1. | .00 37.85 | 6 |
| Alon 2570 O Ela A 570 | 11.201 | 18.930 69 | 9.156 1. | .00 37.95 | 8 |
| • | • | • | | | |

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| | 0.054 | | | | | | | |
|------|-------|-----------|--------|----------|---------------------|--------|------------|----|
| ATOM | 2971 | | A 371 | 11.827 | 20.944 | 68.325 | 1.00 37.78 | 7 |
| ATOM | 2972 | CA ALA | A 371 | 13.264 | 20.704 | 68.340 | 1.00 36.39 | 6 |
| ATOM | 2973 | CB ALA | A 371 | 14.007 | | 68.200 | 1.00 37.73 | 6 |
| ATOM | 2974 | _ | A 371 | | | | | |
| | | | | 13.719 | 19.972 | 69.603 | 1.00 35.42 | 6 |
| ATOM | 2975 | | A 371 | 14.424 | 18.964 | 69.525 | 1.00 32.06 | 8 |
| MOTA | 2976 | N ALA | A 372 | 13.317 | 20.478 | 70.766 | 1.00 33.96 | 7 |
| ATOM | 2977 | CA ALA | A 372 | 13.695 | 19.848 | 72.024 | 1.00 32.22 | |
| | | - | | | | | | 6 |
| MOTA | 2978 | | A 372 | 12.946 | 20.486 | 73.165 | 1.00 28.27 | 6 |
| MOTA | 2979 | C ALA | A -372 | 13.372 | 18.362 | 71.953 | 1.00 31.75 | 6 |
| MOTA | 2980 | O ALA | A 372 | 14.183 | 17.517 | 72.338 | 1.00 31.56 | 8 |
| ATOM | 2981 | | A 373 | - 12.187 | 18.059 | 71.432 | 1.00 32.72 | |
| | | | | | | | | 7 |
| MOTA | 2982 | | A 373 | 11.710 | 16.684 | 71.305 | 1.00 32.32 | 6 |
| MOTA | 2983 | CB ALA | A 373 | 10.206 | 16.689 | 71.103 | 1.00 30.18 | 6 |
| ATOM | 2984 | C ALA | 373 | 12.385 | 15.921 | 70.172 | 1.00 33.13 | 6 |
| MOTA | 2985 | OT1 ALA | 377 | 13.078 | 14.926 | 70.468 | 1.00 35.87 | |
| | | | | | | | | 8 |
| MOTA | 2986 | OT2 ALA | | 12.218 | 16.320 | 69.003 | 1.00 34.11 | 8 |
| ATOM | 2987 | ZN ZN 2 | 951 | 22.693 | 34.497 | 53.990 | 1.00 36.45 | 6 |
| ATOM | 2988 | OH2 WAT S | 3 1 | 35.654 | 44.211 | 49.416 | 1.00 9.27 | 8 |
| ATOM | 2989 | OH2 WAT S | | 24.480 | 33.130 | 53.069 | | |
| | | | | | | | 1.00 21.27 | 8 |
| ATOM | 2990 | OH2 WAT S | | 22.124 | 30.277 | 59.314 | 1.00 14.69 | 8 |
| ATOM | 2991 | OH2 WAT S | 5 4 | 13.839 | 20.611 | 75.741 | 1.00 27.94 | 8 |
| ATOM | 2992 | OH2 WAT S | 5 5 | 34.033 | 41.903 | 46.522 | 1.00 44.54 | 8 |
| MOTA | 2993 | OH2 WAT S | | 15.039 | 42.130 | | | |
| | | | | | • | 55.781 | 1.00 23.79 | 8 |
| ATOM | 2994 | OH2 WAT S | | 32.737 | 41.397 | 75.900 | 1.00 15.80 | 8 |
| ATOM | 2995 | OH2 WAT S | 8 | 11.367 | 22.606 | 58.814 | 1.00 23.37 | 8 |
| ATOM | 2996 | OH2 WAT S | 9 | 13.909 | 18.160 | 65.105 | 1.00 29.93 | 8 |
| ATOM | 2997 | OH2 WAT S | | 29.655 | | | | |
| | | | | | 56.108 | 58.029 | 1.00 50.54 | 8 |
| ATOM | 2998 | OH2 WAT S | | 45.405 | 17.964 | 51.885 | 1.00 9.28 | 8 |
| ATOM | 2999 | OH2 WAT S | 12 | 21.870 | 35.873 | 34.515 | 1.00 32.78 | 8 |
| ATOM | 3000 | OH2 WAT S | 13 | 43.504 | 35.670 | 33.779 | 1.00 28.85 | 8 |
| ATOM | 3001 | OH2 WAT S | | 2.054 | 37.997 | 68.430 | 1.00 40.53 | |
| | 3002 | | | | | | _ | 8 |
| MOTA | | OH2 WAT S | | 49.730 | 28.024 | 55.966 | 1.00 21.42 | -8 |
| ATOM | 3003 | OH2 WAT S | 16 | 47.503 | 32.289 | 34.336 | 1.00 26.13 | 8 |
| ATOM | 3004 | OH2 WAT S | 17 | 6.101 | 26.102 | 64.434 | 1.00 21.69 | 8 |
| ATOM | 3005 | OH2 WAT S | 18 | 10.761 | 46.748 | 45.836 | 1.00 15.79 | 8 |
| | 3006 | | | | | | | |
| ATOM | | OH2 WAT S | | 9.146 | 16.861 | 61.441 | 1.00 16.68 | 8 |
| ATOM | 3007 | OH2 WAT S | 20 | 5.684 | 34.080 | 76.599 | 1.00 37.53 | 8 |
| ATOM | 3008 | OH2 WAT S | 21 | 14.896 | 33.163 | 49.117 | 1.00 34.17 | 8 |
| ATOM | 3009 | OH2 WAT S | 22 | 43.346 | 40.839 | 36.825 | 1.00 35.64 | 8 |
| | 3010 | OH2 WAT S | | | | | | |
| ATOM | | | 23 | 0.516 | 27.705 | 69.174 | 1.00 21.02 | 8 |
| ATOM | 3011 | OH2 WAT S | 24 | 41.270 | 25.444 | 29.717 | 1.00 29.80 | 8 |
| MOTA | 3012 | OH2 WAT S | 25 | 17.818 | 29.142 | 54.584 | 1.00 27.92 | 8 |
| ATOM | 3013 | OH2 WAT S | 26 | 21.512 | 60.572 | 56.912 | 1.00 16.77 | 8 |
| ATOM | 3014 | OH2 WAT S | 27 | 21,211 | | 48.347 | | |
| | | | | | | | 1.00 23.93 | 8 |
| ATOM | 3015 | OH2 WAT S | 28 | 47.805 | 24.638 | 56.619 | 1.00 23.73 | 8 |
| MOTA | 3016 | OH2 WAT S | 25 | 44.624 | 50.302 | 58.154 | 1.00 16.79 | 8 |
| ATOM | 3017 | OH2 WAT S | 3€ | 31.096 | 16.437 | 51.311 | 1.00 26.61 | 8 |
| ATOM | 3018 | OH2 WAT S | 31 | 39.837 | 38.833 | 55.145 | | |
| | | | | | | | 1.00 32.28 | 8 |
| MOTA | 3019 | OH2 WAT S | 32 | 11.660 | 43.601 | 63.704 | 1.00 22.94 | 8 |
| MOTA | 3020 | OH2 WAT S | 33 | 49.899 | 23.474 | 53.058 | 1.00 26.85 | 8 |
| ATOM | 3021 | OH2 WAT S | 34 | 34.624 | 17.734 | 32,228 | 1.00 21.18 | 8 |
| | 3022 | OH2 WAT S | 35 | 26.926 | 15.913 | 62.444 | 1.00 27.01 | |
| ATOM | | | | | | | | 8 |
| MOTA | 3023 | OH2 WAT S | 36 | 8.893 | 28.686 | 63.905 | 1.00 27.68 | 8 |
| ATOM | 3024 | OH2 WAT S | 37 | 23.381 | 26.634 ⁻ | 43.532 | 1.00 24.42 | 8 |
| ATOM | 3025 | OH2 WAT S | 38 | 48.484 | 27.990 | 65.270 | 1.00 34.86 | 8 |
| | 3026 | OH2 WAT S | 39 | 43.382 | | 74.379 | | |
| ATOM | | | | | 28.410 | | 1.00 25.68 | 8 |
| MOTA | 302,7 | OH2 WAT S | 40 | 42.904 | 18.967 | 70.272 | 1.00 29.45 | 8 |
| ATOM | 3028 | OH2 WAT S | 41 | 20.521 | 53.828 | 50.298 | 1.00 22.35 | 8 |
| ATOM | 3029 | OH2 WAT S | 42 | 13.310 | 38.921 | 48.404 | 1.00 23.32 | 8 |
| | | OH2 WAT S | 43 | 9.787 | 46.265 | 60.012 | | |
| ATOM | 3030 | | | | | | 1.00 33.51 | 8 |
| ATOM | 3031 | OH2 WAT S | 44 | 36.089 | 30.416 | 51.377 | 1.00 47.75 | 8 |
| ATOM | 3032 | OH2 WAT S | 45 | 14.831 | 48.131 | 42.151 | 1.00 50.96 | 8 |
| ATOM | 3033 | OH2 WAT S | 46 | 54.162 | 48.194 | 60.971 | 1.00 22.66 | 8 |
| | 3034 | OH2 WAT S | 47 | 38.943 | | 63.509 | 1.00 33.73 | 8 |
| ATOM | | | | | 61.290 | | | |
| ATOM | 3035 | OH2 WAT S | 48 | 29.980 | 18.112 | 33.130 | 1.00 35.80 | 8 |
| ATOM | 3036 | OH2 WAT S | 49 | 31.879 | 50.673 | 44.528 | 1.00 24.39 | 8 |
| •. | | _ | | | | - | | |

| ATOM | 3031 | 7 он2 | WAT : | S 50 | | 39.86 | 53 | 14.629 | 64.30 | 7 1 0 | 0 24.19 | |
|--------------|--------------|------------------|--------|------------|----|--------------------|-----|------------------|------------------|-------|--------------------|------------|
| ATOM | | | | S 51 | | 26.11 | ١9 | 29.471 | | 1.0 | 0 27.78 | 9 8 3 8 |
| ATOM | | | WAT : | | | 48.07 | | 41.589 | 44.011 | 1.0 | 0 36.38 | 3 8 |
| MOTA | | | WAT S | | | 50.80 | | 29.649 | | 1.0 | 0 31.04 | 1 8 |
| MOTA MOTA | | | WAT S | | | 49.54 | | 35.532 | | | 0 20.96 | 5 8 |
| ATOM | _ | | WAT S | | | 6.88 25.69 | | 23.426 | | 1.0 | 0 17.49 | 9 8 |
| ATOM | | | WAT S | | | 45.49 | | 39.891 44.101 | 37.674 55.393 | 1.00 | 51.51 | |
| MOTA | | | WAT S | | | 44.66 | | | | | 37.34 | |
| MOTA | 3046 | OH2 | WAT S | | | 21.91 | | 21.320 | | | 9 44.52 9 26.96 | |
| ATOM | 3047 | | WAT S | 60 | | 27.29 | | 21.016 | | 1.00 | 27.74 | · 8 |
| ATOM | 3048 | | WAT S | _ | | 19.80 | 9 | 49.810 | | | 46.14 | 8 |
| MOTA | 3049 | | WAT S | | - | 30.84 | | 18.035 | | | 42.23 | 8 |
| MOTA | 3050 | | WAT S | | | 19.05 | | 33.379 | | 1.00 | 28.99 | 8. |
| MOTA MOTA | 3051 3052 | | WAT S | | | 47.92 | | 33.253 | 61.470 | | 34.93 | 8 |
| ATOM | 3053 | | WAT S | | | 32.50 27.24 | | 36.000 | 41.000 | | 35.33 | 8 |
| ATOM | 3054 | OH2 | | | | 5.17 | | 56.551 32.914 | 44.579 | 1.00 | 34.19 | |
| ATOM | 3055 | OH2 | | | • | 41.15 | | 51.018 | 54.669 49.348 | 1.00 | 41.89 | _ |
| ATOM | 3056 | OH2 | WAT S | | | 12.869 | | 50.298 | | 1 00 | 31.30 | 8 |
| ATOM | 3057 | OH2 | | 70 | | 17.499 | 9 | 12.826 | 63.854 | | 24.91 | 8 8 |
| ATOM | 3058 | | WAT S | 71 | | 27.152 | | 12.189 | 53.999 | 1.00 | 18.76 | 8 |
| ATOM | 3059 | OH2 | | 72 | | 25.213 | | 54.809 | 67.866 | 1.00 | 61.35 | 8 |
| ATOM ATOM | 3060 3061 | OH2 | WAT S | 73 | | 17.671 | | 48.515 | 53.188 | 1.00 | 37.63 | 8 |
| ATOM | 3062 | | WAT S | 74 75 | | . 23.765 35.535 | | 60.846 | 66.579 | 1.00 | 21.81 | 8 |
| ATOM | 3063 | OH2 | | 76 | | 26.280 | | 27.040 16.065 | 70.698 | | 34.04 | . 8 |
| ATOM | 3064 | OH2 | | 77 | | 18.451 | | 25.555 | 76.564 45.150 | | 32.20 28.55 | 8 |
| ATOM | 3065 | OH2 | WAT S | 78 | | 10.446 | | 61.273 | 48.633 | | 44.74 | 8 |
| MOTA | 3066 | | NAT S | 79 | | 13.256 | i | 24.051 | 73.017 | 1.00 | 35.45 | 8 |
| ATOM | 3067 | | AT S | 80 | | 23.571 | | 13.292 | 69.937 | 1.00 | 49.49 | 8 |
| ATOM | 3068 | | VAT S | 81 | | 29.891 | | 18.071 | 46.109 | 1.00 | 22.84 | 8 |
| MOTA MOTA | 3069 3070 | | VAT S | 82 | | 12.886 | | 42.723 | 75.807 | | 35.31 | 8 |
| ATOM | 3071 | | VAT S | 83 · 84 | | 41.348 | | 15.471 | 45.004 | | 47.24 | 8 |
| ATOM | 3072 | OH2 V | | 85 | | 13.406 30.444 | | 44.647 35.217 | 71.349 | | 49.67 | 8 |
| ATOM | 3073 | OH2 V | | 86 | | 5.217 | | 40.817 | 51.882 61.244 | 1.00 | 38.15 19.51 | 8 |
| ATOM | 3074 | CH2 W | AT S | 87 | | 8.891 | | 21.532 | 56.838 | | 30.72 | 8 8 |
| ATOM | 3075 | OH2 W | | 88 | | 41.816 | | 25.022 | 72.452 | | 22.92 | 8 |
| ATOM | 3076 | OH2 W | | 89 | | 50.621 | | 36.644 | 60.248 | | 29.29 | 8 |
| ATOM | 3077 | OH2 W | | 90 | | 26.008 | | 34.532 | 49.627 | | 45.42 | 8 |
| MOTA MOTA | 3078 3079 | OH2 W | | 91 92 | | 8.131 | | 39.168 | 54.903 | | 31.50 | 8 |
| ATOM | 3080 | OH2 W | | 93 | | 16.591 34.773 | | 58.091 54.065 | 57.551 | | 34.73 | 8 |
| MOTA | 3081 | OH2 W | | 94 | | 42.105 | | 31.720 | 69.382 71.257 | | 36.05 | 8 |
| MOTA | 3082 | OH2 W | | 95 | | 29.684 | | 2.077 | 73.172 | | 35.49 35.17 | 8 |
| ATOM | 3083 | OH2 W | AT S | 96 | *- | 26.411 | | 7.426 | 38.934 | | 41.68 | 8 8 |
| ATOM | 3084 | OH2 W | | 97 | - | 41.183 | 5 | 2.989 | 62.927 | | 50.77 | 8 |
| ATOM | 3085 | OH2 W | | 98 | | 21.167 | | 6.202 | 63.102 | | 33.36 | 8 |
| ATOM | 3086 | OH2 W | | 99 | | 25.060 | | 8.985 | 36.669 | 1.00 | 46.63 | 8 |
| MOTA MOTA | | OH2 W | | | | 37.304 | | 9.027 | 73.722 | 1.00 | | 8 |
| ATOM | 3089 | | | | | 15.911 48.730 | | 4.635 | 39.343 | 1.00 | | 8 |
| ATOM | 3090 | OH2 W | AT S 1 | 03 | | 24.029 | | 5.803 2.997 | 59.572 74.111 | 1.00 | | 8 |
| MOTA | | OH2 W | | | | 42.477 | | 1.773 | 46.986 | 1.00 | | 8 |
| ATOM | | OH2 W | | | | 29.984 | | 2.945 | 31.397 | | 49.05 44.21 | 8 8 |
| MOTA | 3093 | OH2 WA | T S 1 | .06 | | 40.850 | | 6.936 | 31.885 | 1.00 | | 8 |
| MOTA | | OH2 WA | | | | 9.750 | | 2.487 | 48.823 | 1.00 | | 8 |
| MOTA | | OH2 WA | | | | 7.618 | | 0.171 | 58.896 | 1.00 | | 8 |
| MOTA | | OH2 WA | | | | 17.603 | | 3.771 | 59.767 | 1.00 | | 8 |
| | | OH2 WA | | | | 22.590 | | | 67.501 | 1.00 | | 8 |
| ATOM | | OH2 WA | | | | 21.034 | | | 76.056 | 1.00 | | 8 |
| ATOM ATOM | | DH2 WA DH2 WA | | | | 24.791 40.750 | | | 50.081 | 1.00 | | 8 |
| ATOM | | OH2 WA | | | | 7.708 | | | 54.056 58.027 | 1.00 | | 8 |
| MOTA | | H2 WA | - | _ | | 32.375 | | | 77.566 | 1.00 | | 8 |
| | | | | • | | - | -3. | | | 1.00 | | 8 |

| ATOM | 3103 | OH2 WAT S 116 | 5.596 | 17.009 | 64.551 | 1.00 39.15 | 8 |
|--------------|--------------|--------------------------------|------------------|------------------|------------------|--------------------------|---------------------|
| ATOM | 3104 | OH2 WAT S 117 | 20.194 | 5.0.998 | 70.563 | 1.00 19.73 | 8 |
| ATOM | 3105 | OH2 WAT S 118 | 23.853 | 64.927 | 64.164 | 1.00 27.16 | 8 |
| ATOM | 3106 | OH2 WAT S 119 | 9.277 | 43.601 | 46.279 | 1.00 32.31 | 8 |
| ATOM | 3107 | OH2 WAT S 120 | 15.613 | 24.398 | 46.723 | 1.00 55.20 | 8 |
| ATOM | 3108 | OH2 WAT S 121 | 33.110 | 16.122 | 54.229 | 1.00 35.91 | 8 |
| ATOM | 3109 | OH2 WAT S 122 | 26.772 | 34.085 | 33.852 | 1.00 37.49 | 8 |
| ATOM | 3110 | OH2 WAT S 123 | 28.654 | 37.783 | 75.829 | 1.00 47.30 | 8 |
| ATOM | 3111 | OH2 WAT 5 124 | 49.180 | 22.653 | 59.678 | 1.00 37.33 | 8 |
| MOTA | 3112 | OH2 WAT S 125 | 20.561 | 27.788 | 65.975 | 1.00 67.86 | 8 |
| ATOM | 3113 | OH2 WAT S 126 | 34.251 | 13.344 | 57.366 | 1.00 36.18 | 8 |
| MOTA | 3114 | OH2 WAT S 127 | 49.215 | 36.854 | 48.117 | 1.00 33.63 | 8 |
| ATOM | 3115 | OH2 WAT S 128 | 45.826 | 19.588 | 41.601 | 1.00 44.07 | 8 |
| ATOM | .3116 | OH2 WAT S 129 | 18.693 | 56.382 | 64.014 | 1.00 47.77 | 8 |
| ATOM | 3117 | OH2 WAT S 130 | 44.181 | 24,202 | 36.963 | 1.00 32.70 | 8 |
| ATOM | 3118 | OH2 WAT S 131 | 19.160 | 51.901 | 38.133 | 1.00 54.07 | 8 |
| ATOM | 3119 | OH2 WAT S 132 | 16.904 | 36.558 | 48.679 | 1.00 42.21 | 8 |
| MOTA | 3120 | OH2 WAT S 133 | 46.851 | 26.029 | 34.353 | 1.00 56.33 | 8 |
| ATOM | 3121 | OH2 WAT S 134 | 3.925 | 41.533 | 68.647 | 1.00 45.99 | 8 |
| ATOM | 3122 | OH2 WAT S 135 | 44.590 | 38.382 | 78.167 | 1.00 44.50 | 8 |
| ATOM | 3123 | OH2 WAT S 136 | 6.384 | 19.317 | 71.166 | 1.00 28.17 | 8 |
| ATOM | 3124 | OH2 WAT S 137 | 17.982 | 39.823 | 66.487 | 1.00 49.31 | 8 |
| ATOM | 3125 | OH2 WAT S 138 | 8.317 | 22.286 | 61.863 | 1.00 43.42 | 8 |
| ATOM | 3126 | OH2 WAT S 139 | 29.248 | 14.196 | 55.622 | 1.00 35.55 | 8 |
| ATOM | 3127 | OH2 WAT S 140 | 30.377 | 33.180 | 80.320 | 1.00 43.94 | 8 |
| ATOM | 3128 | OH2 WAT S 141 | 41.842 | 32.906 | 27.392 | 1.00 24.82 | 8 |
| MOTA | 3129 | OH2 WAT S 142 | 33.971 | 3.859 | 64.002 | 1.00 41.93 | 8 |
| ATOM | 3130 | OH2 WAT S 143 | 27.314 | 8.087 | 70.916 | 1.00 49.03 | 8 |
| ATOM | 3131 | OH2 WAT S 144 | 4.310 | 39.006 | 64.550 | 1.00 32.70 | 8 |
| ATOM | 3132 | OH2 WAT S 145 | 2.940 | 19.950 | 63.265 | 1.00 33.24 | 8 |
| ATOM | 3133 | OH2 WAT S 146 | 24.134 | 47.625 | 60.121 | 1.00 44.24 | 8 |
| ATOM | 3134 | OH2 WAT S 147 | 25.035 | 53.746 | 42.337 | 1.00 47.82 | 8 |
| MOTA | 3135 | OH2 WAT S 148 | 32.767 | 38.897 | | 1.00 21.86 | 8 |
| MOTA | 3136 | OH2 WAT S 149 | 37.145 | 57.288 | 47.392 | 1.00 36.13 | 8 |
| MOTA | 31:37 | OH2 WAT S 150 | 25.171 | 18.011 | 32.273 | 1.00 38.04 | 8 |
| MOTA | 3138 | OH2 WAT S 151 | 24.054 | 43.182 | 55.583 | 1.00 41.68 | 8 |
| ATOM | 3139 | OH2 WAT S 152 | 27.686 | 64.936 | 52.937 | 1.00 60.62 | 8 |
| ATOM | 3140 | OH2 WAT S 153 | 24.084 | 39.543 | 76.589 | 1.00 22.62 | 8 |
| MOTA | 3141 | OH2 WAT S 154 | 42.110 | 10.159 | 68.662 | 1.00 46.98 | 8 |
| MOTA | 3142 | OH2 WAT S 155 | 9.675 | 22.905 | 75.335 | 1.00 26.45 | 8 |
| ATOM | 3143 | OH2 WAT S 156 | 4.506 | 34.799 | 52.857 | 1.00 33.84 | 8 |
| ATOM | 3144 | OH2 WAT S 157 | 32.583 | 35.051 | 76.446 | 1.00 36.27 | 8 _. 8 |
| ATOM | 3145 | OH2 WAT S 158 | 40.341 29.473 | 58.311 58.378 | 60.390 71.881 | 1.00 54.69 1.00 28.59 | 8 |
| ATOM | 3146 | OH2 WAT S 159 | 11.829 | 60.543 | 56.138 | 1.00 28.55 | 8 |
| ATOM | 3147 | OH2 WAT S 160 | 24.247 | 48.010 | 67.935 | 1.00 56.62 | 8 |
| ATOM | 3148 | OH2 WAT S 161 OH2 WAT S 162 | 12.853 | 33.929 | 77.503 | 1.00 29.88 | 8 |
| ATOM | 3149 3150 | OH2 WAT S 163 | 9.49 | 26.168 | 59.687 | 1.00 15.42 | 8 |
| MOTA | 3151 | OH2 WAT 5 163 | 27.424 | 16.480 | 38.895 | 1.00 36.86 | 8 |
| ATOM | 3152 | OH2 WAT S 165 | 8.512 | 56.634 | 49.614 | 1.00 30.08 | 8 |
| ATOM | 3153 | OH2 WAT S 166 | 30.721 | 13.394 | 57.919 | 1.00 39.47 | 8 |
| ATOM ATOM | 3154 | OH2 WAT S 167 | 49.594 | 38.223 | 73.903 | 1.00 29.50 | 8 |
| • | 3155 | OH2 WAT S 168 | 41.994 | 48.023 | 74.119 | 1.00 38.12 | 8 |
| ATOM ATOM | 3156 | OH2 WAT S 169 | 42.092 | 39.503 | 33.116 | 1.00 24.47 | 8 |
| | 3157 | OH2 WAT S 170 | 34.547 | 12.749 | 38.054 | 1.00 38.65 | 8 |
| ATOM ATOM | 3158 | OH2 WAT S 171 | 15.377 | 60.862 | 50.791 | 1.00 32.82 | 8 |
| ATOM | 3159 | OH2 WAT S 172 | 31.854 | 42.110 | 62.950 | 1.00 42.43 | 8 |
| ATOM | 3160 | OH2 WAT S 173 | 48.743 | 44.073 | 57.626 | 1.00 34.04 | 8 |
| ATOM | 3161 | OH2 WAT S 174 | 8.723 | 50.038 | 42.232 | 1.00 32.87 | 8 |
| ATOM | 3162 | OH2 WAT S 175 | 14.257 | 18.280 | 53.455 | 1.00 40.51 | 8 |
| ATOM | 31.63 | OH2 WAT S 176 | 31.917 | 37.509 | 53.943 | 1.00 40.43 | 8 |
| ATOM | 3164 | OH2 WAT S 177 | 23.921 | 47.029 | 70.642 | 1.00 47.97 | 8 |
| ATOM | 3165 | OH2 WAT S 178 | 27.974 | 47.778 | 69.949 | 1.00 62.12 | 8 |
| ATOM . | 3166 | OH2 WAT S 179 | 7.850 | 25.093 | 51.345 | 1.00 50.13 | 8 |
| ATOM | 3167 | OH2 WAT S 180 | 22.080 | 48.840 | 66.463 | 1.00 53.81 | 8 |
| MOTA | 3168 | OH2 WAT S 181 | 34.780 | 48.220 | 77.419 | 1.00 30.86 | 8 |

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Figure 17-49

| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 3169 3170 3171 3172 3173 3174 3175 3176 3177 3180 3181 3182 3183 3184 3185 3188 3189 3190 3191 3192 | OH2 WAT S 182 OH2 WAT S 183 OH2 WAT S 184 OH2 WAT S 185 OH2 WAT S 186 OH2 WAT S 187 OH2 WAT S 189 OH2 WAT S 190 OH2 WAT S 190 OH2 WAT S 191 OH2 WAT S 192 OH2 WAT S 194 OH2 WAT S 195 OH2 WAT S 196 OH2 WAT S 197 OH2 WAT S 200 OH2 WAT S 201 OH2 WAT S 201 OH2 WAT S 202 OH2 WAT S 202 OH2 WAT S 204 OH2 WAT S 204 OH2 WAT S 204 OH2 WAT S 204 | 29.166 51.175 18.520 44.774 30.770 22.157 11.778 31.339 31.165 39.705 3.668 25.256 47.575 32.017 35.476 12.180 37.133 40.268 25.159 24.593 36.741 10.013 | 35.526 21.424 51.545 46.208 30.219 9.460 39.535 50.526 60.910 14.244 15.398 34.304 9.360 17.667 13.045 7.006 16.270 21.226 15.712 17.768 27.104 20.267 53.930 16.731 | 52.018 28.950 62.599 42.323 38.653 69.837 78.736 68.987 70.464 72.937 67.925 48.773 34.633 64.436 56.288 75.963 48.199 46.858 65.727 33.858 65.727 33.858 65.727 | 1.00 47.14 1.00 45.08 1.00 33.88 1.00 50.85 1.00 45.36 1.00 37.01 1.00 41.34 1.00 27.47 1.00 47.05 1.00 39.82 1.00 40.79 1.00 47.22 1.00 49.59 1.00 49.88 1.00 49.88 1.00 49.88 1.00 41.90 1.00 41.90 1.00 48.06 1.00 47.07 | *********************** |
|--|--|---|---|---|--|--|-------------------------|
| | | | 35.476 | 7.006 | 64.436 | 1.00 49.59 | |
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| | | | | | | | |
| | 3193 | OH2 WAT S 205 | | 34.778 | 74.101 | 1.00 27.07 | 8 |
| MOTA MOTA | 3194 | OH2 WAT 5 200 | | 55.767 | 45.193 | 1.00 59.49 | 8 |
| MOTA | 3195 | OH2 WAT S 208 | | 18.151 | 36.382 | 1.00 45.31 | 8 |
| ATOM | 3196 | OH2 WAT S 209 | 6.823 | 37.405 | 51.989 | 1.00 58.23 | 8 |
| ATOM | 3197 | OH2 WAT S 210 | | 43.551 | 36.157 | 1.00 30.78 | 8 |
| ATOM | 3198 | OH2 WAT S 211 | 17.038 | 52.360 | 63.283 | 1.00 34.08 | 8 |
| ATOM | 3199 | OH2 WAT S 212 | 30.001 | 18.471 | 49.568 | .1.00 33.92 | 8 |
| ATOM | 3200 | OH2 WAT S 213 | 23.045 | 28.615 | 33.729 | 1.00 44.22 | 8 |
| ATOM | 3201 | OH2 WAT S 214 | 26.130 | 61.496 | 75.246 | 1.00 40.49 | 8 |
| MOTA | 3202 | OH2 WAT S 215 | 33.881 | 32.473 | 46.604 | 1.00 39.35 | 8 |
| ATOM | 3203 | OH2 WAT S 216 | 23.887 | 45.987 | 44.362 | 1.00 36.50 | 8 |
| ATOM | 3204 | OH2 WAT S 217 | 6.925 | 42.281 | 65.917 | 1.00 34.22 | 8 |
| atom End | 3205 | OH2 WAT S 218 | 32.823 | 8.977 | 59.213 | 1.00 27.03 | 8 |

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| | | | | | 11//26 | 3 | |
|-------|----|------|--------|------------|-----------|----------------|--------------------------|
| | | | | | Figure 13 | 8-1 | |
| | | | | Resid | due # X | Y Z | B Segment ID |
| ATOM | 1 | . CB | ALA | | 46.726 | | 1.00 56.80 |
| ATOM | 2 | C | ALA | | 47.943 | | 1.00 58.93 |
| ATOM | 3 | 0 | ALA | | 48.857 | | 1.00 60.99 |
| ATOM | 4 | N | ALA | | 46.995 | | 1.00 56.88 |
| ATOM | 5 | CA | ALA | | 46.801 | | 1.00 59.41 |
| ATOM- | 6 | | LYS | | 47.890 | | 1.00 53.81 |
| ATOM | 7 | | LYS | | 48.937 | | 1.00 53.62 |
| ATOM | 8 | | LYS | | 48.736 | | 1.00 50.26 |
| MOTA | 9 | - | LYS | | 48.917 | | |
| ATOM | 10 | | LYS | | 48.950 | | 1.00 56.64 1.00 57.18 |
| ATOM | 11 | | LYS | | 49.160 | | |
| MOTA | 12 | | LYS | | 50.423 | | 1.00 56.74 |
| MOTA | 13 | | LYS | | 49.063 | | 1.00 54.86 |
| ATOM | 14 | | LYS | | 48.088 | 10.562 136.248 | 1.00 49.95 |
| MOTA | 15 | | VAL | | 50.287 | 10.147 136.550 | 1.00 44.34 |
| ATOM | 16 | | VAL | | 50.609 | 9.985 135.142 | 1.00 46.01 |
| ATOM | 17 | | VAL | | 51.901 | 10.755 134.809 | 1.00 42.48 |
| ATOM | 18 | | L VAL | | 52.179 | 10.713 134.809 | 1.00 43.42 |
| ATOM | 19 | | VAL A | | 51.773 | 12.186 135.310 | 1.00 39.20 |
| ATOM | 20 | C | VAL | | 50.787 | 8.510 134.806 | 1.00 39.34 |
| MOTA | 21 | ō | VAL | | 51.659 | 7.839 135.351 | 1.00 38.41 |
| ATOM | 22 | N | LYS | | 49.959 | 8.011 133.899 | 1.00 37.08 |
| ATOM | 23 | CA | LYS A | | 50.016 | 6.610 133.515 | 1.00 37.79 |
| ATOM | 24 | CB | LYS A | | 48.700 | 5.915 133.887 | 1.00 38.17 |
| ATOM | 25 | CG | LYS A | | 48.411 | 5.803 135.385 | 1.00 38.40 |
| ATOM | 26 | CD | LYS A | . 5 . 5 | 49.384 | 4.855 136.070 | 1.00 42.84 |
| ATOM | 27 | CE | LYS A | | 49.017 | 4.632 137.534 | 1.00 44.10 |
| ATOM | 28 | NZ | LYS A | | 49.045 | 5.894 138.322 | 1.00 45.97 |
| ATOM | 29 | C | LYS 3 | | 50.275 | 6.392 132.030 | 1.00 51.78 |
| ATOM | 30 | ō | LYS A | | 49.992 | 7.253 131.201 | 1.00 38.31 1.00 38.13 |
| ATOM | 31 | N | LEU A | | 50.817 | 5.220 131.717 | |
| ATOM | 32 | CA | LEU A | | 51.082 | 4.818 130.346 | 1.00 35.05 1.00 31.46 |
| MOTA | 33 | СВ | LEU A | | 52.582 | 4.592 130.133 | 1.00 28.46 |
| ATOM | 34 | CG | LEU A | | 53.094 | 4.256 128.720 | 1.00 28.46 |
| ATOM | 35 | | LEU A | | 52.618 | 2.884 128.295 | 1.00 33.05 |
| ATOM | 36 | CD2 | | | 52.630 | 5.312 127.744 | 1.00 21.96 |
| ATOM | 37 | C | LEU A | | 50.307 | 3.512 130.164 | 1.00 30.50 |
| ATOM | 38 | 0 | LEU A | | 50.453 | 2.581 130.955 | 1.00 32.82 |
| ATOM | 39 | N | ILE A | | 49.459 | 3.456 129.145 | 1.00 26.94 |
| ATOM | 40 | CA | ILE A | | 48.676 | 2.255 128.893 | 1.00 28.29 |
| MOTA | 41 | CB | ILE A | | 47.218 | 2.598 128.493 | 1.00 28.94 |
| MOTA | 42 | CG2 | | | 46.499 | 1.343 128.041 | 1.00 32.57 |
| ATOM | 43 | CG1 | ILE A | . 7 | 46.447 | 3.172 129.688 | 1.00 36.59 |
| MOTA | 44 | CD1 | ILE A | . 7 | 46.979 | 4.468 130.236 | 1.00 46.80 |
| MOTA | 45 | С | ILE A | . 7 | 49.341 | 1.470 127.770 | 1.00 31.09 |
| MOTA | 46 | 0 | IL" A | | 49.600 | 2.009 126.695 | 1.00 27.65 |
| MOTA | 47 | N | ·GL: A | . 8 | 49.638 | 0.201 128.029 | 1.00 27.30 |
| MOTA | 48 | CA | GL' A | . 8 | 50.277 | -0.614 127.016 | 1.00 25.50 |
| MOTA | 49 | С | GLY A | 8 | 50.578 | -2.024 127.480 | 1.00 30.66 |
| ATOM | 50 | 0 | GLY A | 8 | 50.224 | -2.421 128.592 | 1.00 30.02 |
| ATOM | 51 | N | THR A | 9 | 51.238 | -2.777 126.611 | 1.00 28.94 |
| MOTA | 52 | CA | THE A | 9 | 51.614 | -4.156 126.877 | 1.00 33.63 |
| ATOM | 53 | CB | THR A | 9 | 50.393 | -5.083 126.857 | 1.00 36.19 |
| MOTA | 54 | OG1 | THR A | 9 | 50.827 | -6.441 126.992 | 1.00 34.87 |
| MOTA | 55 | CG2 | THR A | 9 | 49.633 | -4.931 125.548 | 1.00 36.49 |
| MOTA | 56 | C | THR A | 9 | 52.567 | -4.637 125.794 | 1.00 34.83 |
| MOTA | 57 | 0 | THR A | 9 | 52.545 | -4.133 124.677 | 1.00 36.91 |
| ATOM | 58 | N | LEU A | 10 | 53.407 | -5.609 126.129 | 1.00 39.15 |
| ATOM | 59 | CA | LEU A | 10 | 54.345 | -6.167 125.164 | 1.00 40.21 |
| ATOM | 60 | CB | LEU A | 10 | 55.402 | -7.009 125.881 | 1.00 42.40 |
| ATOM | 61 | CG | LEU A | 10 | 56.482 | ~6.282 126.687 | 1.00 42.29 |
| ATOM | 62 | | LEU A | 10 | 55.870 | -5.293 127.647 | 1.00 42.92 |
| ATOM | 63 | CD2 | LEU Á | 10 | 57.319 | -7.306 127.424 | 1.00 40.29 |
| ATOM | 64 | С | LEU A | 10 | 53.591 | -7.039 124.159 | 1.00 41.70 |
| ATOM | 65 | 0 | LEU A | 10 | 54.055 | -7.266 123.044 | 1.00 37.13 |
| ATOM | 66 | N | ASP A | 11 | 52.419 | -7.519 124.557 | 1.00 47.28 |
| | | | • | | | | |

| ATOM | 61 | 7 CA | ASP | A 11 | 51.617 | -8.36 | 9 123.683 | 1.00 53.30 |
|--------------|-----|--------|---------|------|----------------|---------|------------------------|------------|
| ATOM | 68 | | | | 50.230 | -8.60 | 8 124.287 | 1.00 52.35 |
| ATOM | 69 | | | | 50.295 | -9 33 | 1 125.610 | |
| ATOM | 70 | | _ | A 11 | | -10.35 | 1 123.010 0 125 605 | |
| MOTA | 71 | | | | 49.630 | _8 00 | 8 125.685 3 126.567 | |
| ATOM | 72 | | | | | 7 04 | 3 126.36/ | |
| | | _ | ASP | | 51.459 | -7.84 | 0 122.257 | |
| MOTA | 73 | - | ASP . | | 51.360 | -8.62 | 6 121.311 | 1.00 54.31 |
| MOTA | 74 | | TYR | | 51.424 | -6.52 | 1 122.092 | |
| MOTA | 75 | | | | 51.275 | | 0 120.749 | 1.00 51.41 |
| ATOM | 76 | | | A 12 | 51.328 | | | 1.00 49.05 |
| ATOM | 77 | | | | 50.164 | -3.72 | 9 121.421 | 1.00 45.48 |
| MOTA | 78 | | l Tyr . | | 50.296 | -3.15 | 7 122.686 | 1.00 47.08 |
| ATOM | 79 | CE | 1 TYR . | A 12 | 49.252 | -2.43 | 0 123.263 | 1.00 47.53 |
| ATOM | 80 | CD | 2 TYR 2 | A 12 | 48.952 | -3.56 | 5 120.749 | 1.00 43.77 |
| MOTA | 81 | CE | 2 TYR 2 | A 12 | 47.906 | -2.84 | | 1.00 44.16 |
| ATOM | 82 | CZ | TYR A | A 12 | 48.061 | -2.279 | 122.566 | 1.00 48.67 |
| ATOM | 83 | OH | TYR A | | 47.030 | -1.548 | 3 123.116 | 1.00 48.65 |
| ATOM | 84 | С | TYR A | | 52.367 | -6.503 | 3 119.816 | 1.00 50.01 |
| ATOM | 85 | 0 | TYR A | | 52.197 | -6.525 | 118.596 | 1.00 45.56 |
| ATOM | 86 | N | GLY A | | 53.484 | -6 931 | 120.396 | 1.00 48.72 |
| ATOM | 87 | CA | GLY A | | 54.574 | | 119.599 | 1.00 50.56 |
| ATOM | 88 | c | GLY A | | 54.196 | | 118.857 | 1.00 53.32 |
| ATOM | 89 | ŏ | GLY A | | 54.931 | | 117.982 | 1.00 52.64 |
| ATOM | 90 | . N | LYS A | | 53.045 | | 119.207 | |
| ATOM | 91 | CA | LYS A | | | | 113.207 | 1.00 53.37 |
| ATOM | 92 | CB | LYS A | | 52.333 | -10.316 | 119.653 | 1.00 54.56 |
| ATOM | 93 | CG | LYS A | | 52.022 | -11.4/ | 120.591 | 1.00 58.02 |
| ATOM | 94 | CD | LYS A | | 53.000 | 12.002 | 119.918 | 1.00 62.81 |
| ATOM | 95 | CE | LYS A | | 54 747 | 13.134 | 119.918 | 1.00 61.61 |
| ATOM | 96 | NZ | LYS A | | 56.797 | 12 712 | 118.734 | 1.00 61.77 |
| ATOM | 97 | | | | | | | 1.00 58.35 |
| ATOM | 98 | C O | LYS A | | | | 117.559 | 1.00 52.03 |
| | 99 | | LYS A | | | | 116.942 | 1.00 51.71 |
| ATOM | | N | TYR A | | 51.143 | | .117.372 | 1.00 46.92 |
| ATOM | 100 | CA | TYR A | | 50.091 | | 116.449 | 1.00 47.99 |
| ATOM | 101 | CB | TYR A | | 48.959 | | 117.253 | 1.00 50.40 |
| ATOM | 102 | CG | TYR A | | 48.456 | -8.793 | | 1.00 53.01 |
| ATOM | 103 | CD1 | | | 48.166 | | 119.637 | 1.00 52.10 |
| ATOM | 104 | CE1 | | 15 | 47.722 | | 120.685 | 1.00 51.72 |
| MOTA | 105 | CD2 | | 15 | | | 118.208 | 1.00 54.67 |
| ATOM | 106 | CE2 | | 15 | | ~10.976 | | 1.00 55.69 |
| ATOM | 107 | CZ | TYR A | 15 | 47.561 | | | 1.00 54.18 |
| MOTA | 108 | OH | TYR A | 15 | | | 121.520 | 1.00 55.42 |
| ATOM | 109 | C | TYR A | 15 | 50.592 | | 115.353 | 1.00 46.20 |
| ATOM | 110 | 0 | TYR A | 15 | 49.933 | | 115.018 | 1.00 43.72 |
| ATOM | 111 | N | ARG A | 16 | 51.758 | | 114.791 | 1.00 46.29 |
| MOTA | 112 | CA | ARG A | 16 | 52.347 | | 113.727 | 1.00 45.66 |
| MOTA | 113 | CB | ARG A | 16 | 53.779 | -7.545 | | 1.00 50.56 |
| ATOM | 114 | CG | ARG A | 16 | 54.677 | | 114.636 | 1.00 56.90 |
| MOTA | 115 | CD | ARG A | | 54.992 | | 115.315 | 1.00 60.72 |
| ATOM | 116 | NE | ARG A | 16 | 56.021 | | 116.328 | 1.00 66.70 |
| Mota | 117 | CZ | ARG A | 16 | 5 7.211 | -7.141 | 116.070 | 1.00 66.68 |
| MOTA | 118 | | ARG A | 16 | 57.520 | -7.519 | 114.834 | 1.00 65.68 |
| atom | 119 | | ARG A | 16 | 58.093 | -7.314 | 117.046 | 1.00 66.33 |
| MOTA | 120 | С | ARG A | 16 | 51.573 | | 112.429 | 1.00 44.20 |
| ATOM | 121 | 0 | ARG A | 16 | 50.871 | -8.293 | 112.254 | 1.00 43.41 |
| MOTA | 122 | N | TYR A | 17 | 51.715 | | 111.514 | 1.00 39.23 |
| ATOM | 123 | CA | TYR A | 17 | 51.067 | -6.453 | 110.215 | 1.00 38.71 |
| ATOM | 124 | CB | TYR A | 17 | 50.913 | | 109.565 | 1.00 33.83 |
| ATOM . | 125 | CG | TYR A | 17 | 49.744 | | 110.084 | 1.00 27.35 |
| ATOM | 126 | CD1 | TYR A | 17 | 49.598 | | 111.443 | 1.00 27.25 |
| ATOM | 127 | CE1 | TYR A | 17 | 48.540 | | 111.909 | 1.00 27.16 |
| ATOM | 128 | | TYR A | 17 | 48.807 | | 109.204 | 1.00 25.78 |
| ATOM | 129 | CE2 | TYR A | 17 | 47.752 | -2.925 | | 1.00 26.34 |
| ATOM | 130 | CZ | TYR A | 17 | 47.626 | | 111.009 | 1.00 27.28 |
| atom atom | 131 | OH | TYR A | 17 | 46.602 | | 111.450 | 1.00 27.20 |
| ATOM ATOM | 132 | | TYR A | 17 | 51.972 | | 109.368 | 1.00 41.52 |
| A1011 | | - | · · · | | | | _00.500 | |

| ATOM | 13 | 3 0 | TYR | A 17 | | 53.15 | 0 -7.5 | 25 109.68 | 3 1 00 25 62 |
|--------------|------------|----------|----------------|----------|---|------------------|------------------|--------------------|--------------------------|
| MOTA | 13 | 4 N | | | | 51.44 | | | |
| MOTA | 13 | | D PRO | A 18 | | 50.07 | | | |
| MOTA | 13 | | A PRO | | | 52.20 | | | |
| ATOM | 13 | | B PRO | | | 51.21 | 3 -9.09 | | |
| ATOM | 13 | | G PRO | | | 50.34 | 3 -7.83 | | |
| ATOM | 13 | _ | | | | 53.55 | 6 -8.30 | 3 106.889 | |
| ATOM | 14 | | | | | 53.788 | | | 1.00 49.33 |
| MOTA | 14 | _ | | | | 54.432 | 2 -9.26 | 106.592 | |
| ATOM | 14 | _ | | | | 55.800 | | | 1.00 57.00 |
| ATOM ATOM | 14: 14: | _ | | | | 56.223 | | | |
| ATOM | 14: | | | A 19 | | | -10.92 | | |
| MOTA | 140 | | | | | 54.239 | | | |
| ATOM | 14 | | | | | | -10.65 | | |
| ATOM | 148 | | | A 19 | | 52.116 56.229 | | | |
| ATOM | 149 | | | A 19 | ` | 57.230 | | | |
| ATOM | 150 | | | A 20 | | 55.515 | | | |
| ATOM | 151 | L CF | | | | 55.925 | | | |
| ATOM | 152 | CE | | A 20 | | 55.829 | | | 1.00 50.02 |
| ATOM | 153 | CG | ASN A | A 20 | | 56.729 | | | |
| ATOM | 154 | | 1 ASN 2 | A 20 | | 57.948 | | | 1.00 46.88 |
| ATOM | 155 | | 2 ASN A | A 20 | | 56.130 | | | 1.00 50.85 |
| ATOM | 156 | | ASN A | | | 55.167 | -4.86 | | 1.00 45.50 |
| ATOM | 157 | | ASN A | | | 55.481 | -3.77 | | 1.00 45.35 |
| MOTA | 158 | | HIS A | | | 54.182 | -4.99 | | 1.00 37.46 |
| ATOM ATOM | 159 160 | | | | | 53.374 | -3.86 | | 1.00 32.39 |
| ATOM | 161 | CG | | | | 52.198 | -4.35! | | 1.00 29.34 |
| ATOM | 162 | | 2 HIS A | | | 51.118 50.999 | -3.339 | | 1.00 30.50 |
| ATOM | 163 | | 1 HIS A | | | 49.993 | -2.314 -3.298 | | 1.00 22.88 |
| ATOM | 164 | | 1 HIS A | | | 49.226 | -2.293 | | 1.00 30.15 1.00 30.96 |
| ATOM | 165 | NE. | 2 HIS A | | | 49.814 | -1.680 | | 1.00 36.41 |
| ATOM | 166 | C | HIS A | | | 54.194 | -2:879 | | 1.00 29.18 |
| ATOM | 167 | 0 | HIS A | | | 55.030 | -3.279 | | 1.00 26.92 |
| ATOM | 168 | N | PRO A | | | 53.965 | -1.572 | 105.969 | 1.00 31.12 |
| ATOM | 169 | CD | PRO A | | | 53.027 | -0.912 | | 1.00 29.46 |
| MOTA MOTA | 170 171 | CA CB | PRO A | | | 54.702 | -0.567 | | 1.00 29.27 |
| ATOM | 172 | CG | PRO A PRO A | 22 22 | | 54.012 | 0.732 | | 1.00 26.00 |
| ATOM | 173 | c | PRO A | 22 | | 53.670 54.624 | 0.434 | | 1.00 31.52 |
| ATOM | 174 | ō | PRO A | 22 | | 55.575 | -0.822 -0.538 | | 1.00 29.96 |
| ATOM | 175 | N | LEU A | 23 | | 53.501 | -1.371 | | 1.00 27.47 |
| ATOM | 176 | CA | LEU A | 23 | | 53.309 | -1.644 | | 1.00 26.64 1.00 30.44 |
| MOTA | 177 | CB | LEU A | 23 | | 51.833 | -1.428 | | 1.00 24.09 |
| MOTA | 178 | CG | LEU A. | 23 | | 51.356 | 0.029 | _ | 1.00 25.30 |
| ATCM | 179 | | LEU A | 23 · | | 49.836 | 0.103 | 110.668 | 1.00 17.72 |
| MCTA | 180 | | LEU A | 23 | | 52.086 | 0.816 | 111.574 | 1.00 24.15 |
| ATOM | 181 | C | LEU A | 23 | | 53.775 | -3.015 | 110.662 | 1.00 31.64 |
| ATCM | 182 183 | NO | LEU A | 23 | | 53.252 | -3.512 | 111.667 | 1.00 31.00 |
| atom atom | 184 | CA | LYS A | 24 | | 54.753 | | 110.012 | 1.00 28.25 |
| ATOM | 185 | CB | LYS A | 24 24 | | 55.200 55.718 | | 110.513 | 1.00 30.90 |
| ATOM | 186 | CG | LYS A | 24 | | 57.178 | | 109.372 108.982 | 1.00 36.59 |
| ATOM | 187 | CD | LYS A | 24 | | 57.546 | | 108.535 | 1.00 40.77 |
| ATOM | 188 | CE | LYS A | 24 | | 58.858 | _ | 107.755 | 1.00 44.61 |
| ATOM | 189 | NZ | LYS A | 24 | | 59.959 | | 108.487 | 1.00 50.44 1.00 51.30 |
| MOTA | 190 | С | LYS A | 24 | | 56.282 | | 111.581 | 1.00 32.57 |
| MOTA | 191 | 0 | LYS A | 24 | | 56.695 | | 112.245 | 1.00 29.83 |
| MCTA | 192 | N | ILE A | 25 | | 56.729 | | 111.750 | 1.00 27.06 |
| atom | 193 | CA | ILE A | 25 | | 57.755 | -3.200 | 112.739 | 1.00 30.45 |
| ATOM | 194 | CB | ILE A | 25 | | 58.416 | | 112.499 | 1.00 33.37 |
| atom | 195 | CG2 | | 25 | | 59.056 | | 111.120 | 1.00 33.22 |
| ATOM · | 196 | CG1 | ILE A | 25 | | 57.361 | | 112.662 | 1.00 30.45 |
| | 197 | | ILE A | 25 25 | | 57.930 | | 112.700 | 1.00 33.12 |
| ATCM | 198 | С | ILE A | 25 | | 57.156 | -3.129 | 114.141 | 1.00 32.10 |

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Figure 18-4

| | | | • | | | | |
|--------|----------------|------|--------|---------|-----------|------------------|--------------|
| MOTA | 199 O ILE | A 25 | 55.967 | 7 -2.85 | 1 114.310 | 1.00 2 | 00 15 |
| ATOM | 200 N PBO | | 57.979 | | 2 115.168 | | 1.64 |
| MOTA | 201 CD PRO | | 59.395 | | 8 115.139 | | 1.11 |
| ATOM | 202 CA PRO | | 57.507 | 7 -3 32 | 2 116.556 | 1.00 3 | |
| MOTA | 203 CB PRO | _ | 58.709 | | 0 117.347 | | 17.04 |
| ATOM | 204 CG PRO | | 59.454 | | 1 116.324 | | |
| MOTA | 205 C PRO | | 57.265 | | 0 116.827 | | |
| MOTA | 206 O PRO | | 58.001 | | 4 116.315 | | 8.42 |
| MOTA | 207 N ARG | | 56.251 | | 4 117.614 | | 4 10 |
| ATOM | 208 CA ARG | | 55.977 | | 6 117.899 | | 8.53 |
| ATOM | 209 CB ARG | | 54.787 | | 8 117:048 | | |
| ATOM | 210 CG ARG | | 55.075 | | 115.554 | | 9.77 |
| ATOM | 211 CD ARG | | 53.918 | | 3 114.620 | | 9.64 6.61 |
| ATOM | 212 NE ARG | | 53.622 | | 5 114.517 | | |
| ATOM | 213 CZ ARG | | 52.649 | | 115.173 | 1.00 2 1.00 2 | 0.54 |
| ATOM | | A 27 | 51.857 | | 115.999 | 1.00 2 | 9.70 |
| ATOM | 215 NH2 ARG | | 52.451 | | 114.983 | 1.00 3 | 0.1/ |
| MOTA | 216 C ARG | | 55.746 | | 119.387 | 1.00 2 | |
| MOTA | 217 O ARG | | 56.679 | | 120.113 | 1.00 2 | 4.60 |
| ATOM | 218 N VAL | | 54.529 | -0.117 | | | |
| ATOM | 219 CA VAL | | 54.282 | 0.093 | | 1.00 2 1.00 2 | |
| ATOM | 220 CB VAL | | 52.800 | | 121.635 | | |
| ATOM | 221 CG1 VAL | | 52.599 | | 123.142 | 1.00 3 | |
| ATOM | 222 CG2 VAL | | 51.947 | | 120.903 | 1.00 3 | |
| ATOM | 223 C VAL 2 | | 55.158 | | 122.145 | 1.00 3 | |
| ATOM | 224 O VAL 2 | | 55.673 | | 123.182 | 1.00 3 | 2./5 |
| ATOM | 225 N SER 2 | | 55.341 | | 121.718 | 1.00 3 | |
| ATOM | 226 CA SER A | | 56.162 | -2.982 | | 1.00 3 | |
| ATOM | 227 CB SER 2 | | 56.058 | -4.399 | | | 5.92 |
| ATOM | 228 OG SER A | | 56.562 | | 120.579 | | 3.85 |
| ATOM | 229 C SER - A | | 57.609 | -2.482 | | | 1.77 |
| ATOM | 230 O SER A | | 58.378 | | 123.391 | 1.00 29 | |
| ATOM | 231 N LEU A | 30 | 57.967 | | 121.380 | | .20 |
| ATOM | 232 CA LEU A | 30 | 59.317 | -1:234 | | 1.00 32 | |
| ATOM | 233 CB LEU A | 30 | 59.554 | | 119.829 | 1.00 30 | |
| ATOM | 234 CG LEU A | 30 | 61.008 | | 119.333 | 1.00 33 | |
| ATOM | 235 CD1 LEU A | 30 | 61.066 | 0.484 | 118.224 | 1.00 28 | |
| MOTA | 236 CD2 LEU A | 30 | 61.948 | -0.135 | 120.441 | 1.00 35 | |
| MOTA | 237 C LEU A | . 30 | 59.423 | -0.089 | 122.236 | 1.00 30 | |
| ATOM . | 238 O LEU A | | 60.397 | 0.019 | 122.984 | 1.00 27 | |
| ATOM | 239 N LEU A | | 58.408 | 0.769 | 122.232 | 1.00 27 | .38 |
| MOTA | 240 CA LEU A | 31 | 58.372 | 1.915 | 123.126 | 1.00 24 | |
| ATOM | 241 CB LEU A | 31 | 57.008 | 2.596 | 123.042 | 1.00 24 | .92 |
| MOTA | 242 CG LEU A | 31 | 56.918 | 4.069 | 123.460 | 1.00 30 | .49 |
| ATOM | 243 CD1 LEU A | 31 | 55.492 | 4.390 | 123.881 | 1.00 24 | .71 |
| MOTA | 244 CD2 LEU A | 31 | 57.851 | 4.355 | 124.603 | 1.00 27 | .32 |
| MOTA | 245 C LEU A | 31 | 58.610 | 1.429 | 124.564 | 1.00 28 | .18 |
| ATOM | 246 O LEU A | 31 | 59.489 | 1.928 | 125.263 | 1.00 33 | .64 |
| MOTA | 247 N LEU A | 32 | 57.831 | 0.445 | 125.000 | 1.00 30 | .17 |
| ATOM | 248 CA LEU A | 32 | 57.965 | | 126.357 | 1.00 30 | .59- |
| MOTA | 249 CB LEU A | 32 | 56.944 | | 126.601 | 1.00 30 | . 55 |
| ATOM | 250 CG LEU A | 32 | 55.458 | | 126.402 | 1.00 29 | .50 |
| MOTA | 251 CD1 LEU A | 32 | 54.611 | | 126.727 | 1.00 28 | |
| MOTA | .252 CD2 LEU A | 32 | 55.058 | | 127.287 | 1.00 31 | .92 |
| MOTA | 253 C LEU A | 32 | 59.376 | | 126.657 | 1.00 33 | |
| MOTA | 254 O LEU A | 32 | 59.961 | | 127.682 | 1.00 36 | .51 |
| ATOM | 255 N ARG A | 33 | 59.926 | | 125.777 | 1.00.29 | |
| ATOM | 256 CA ARG A | 33 - | 61.271 | | 125.999 | 1.00 33 | . 49 |
| MOTA | 257 CB ARG A | 33 | 61.630 | | 124.945 | 1.00 39 | |
| ATOM | 258 CG ARG A | 33 | 60.814 | | 125.024 | 1.00 44 | |
| MOTA | 259 CD ARG A | 33 | 61.237 | | 123.933 | 1.00 53 | |
| MOTA | 260 NE ARG A | 33 | 60.515 | | 124.007 | 1.00.56 | _ |
| ATOM | 261 CZ ARG A | 33 | 60.611 | -7.384 | 125.014 | 1.00 58 | |
| ATOM | 262 NH1 ARG A | 33 | 61.402 | -7.121 | 126.045 | 1.00 59 | |
| MOTA | 263 NH2 ARG A | 33 | 59.911 | -8.511 | | 1.00 57 | |
| ATOM | 264 C ARG A | 33 | 62.314 | -0.845 | 125.978 | 1.00 31. | 45 |
| | | | | | | | |

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Figure 18-5

| MOTA | 265 O ARG A 33 | 6 | 3.288 | 0.00 | | _ | |
|--------|-------------------|-------|-------|---------|-----------|---------|--------|
| ATOM | | | | -0.88 | 5 126.72 | 2 1.00 | 26.49 |
| | 200 11 1111 17 24 | 6. | 2.103 | 0.14 | 6 125.12 | 3 1.00 | 32.42 |
| ATOM | Ja | 6: | 3.042 | 1.25 | 3 125.00 | | 33.37 |
| ATOM | 268 CB PHE A 34 | | 2.617 | | | | , 33.3 |
| ATOM | 269 CG PHE A 34 | | | 2.10 | 0 123.85 | | 31.68 |
| ATOM | | | 3.653 | 3.20 | | 6 1.00 | 29.05 |
| | | 64 | 1.825 | 2.81 | 9 122.83 | R I no | 29.21 |
| ATOM | 271 CD2 PHE A 34. | 63 | 3.458 | 4.54 | 6 123.78 | | 23.21 |
| MOTA | 272 CE1 PHE A 34 | | .793 | 3.76 | | | 28.25 |
| ATOM | 273 CE2 PHE A. 34 | | | | | | 29.35 |
| ATOM | 274 CZ PHE A 34 | | .416 | 5.50 | | 5 1.00 | 32.67 |
| | 11 J 2 | 65 | .589 | 5.10 | 8 122.783 | | 29.08 |
| ATOM | 275 C PHE A 34 | 63 | .083 | 2.042 | | | 29.00 |
| ATOM | 276 O PHE A 34 | | .155 | | 1 120.30 | | 33.47 |
| ATOM | 0.00 | • | | 2.294 | | | 27.49 |
| ATOM | | | .912 | 2.432 | 2 126.802 | 1.00 | 29.34 |
| | 278 CA LYS A 35 | 61 | .848 | 3.191 | 128.042 | | 31.48 |
| MOTA | 279 CB LYS A 35 | | .406 | 3.576 | | 1.00 | 31.48 |
| ATOM | '280 CG LYS A 35 | | .803 | | | | 30.82 |
| ATOM | | | | 4.552 | | | 32.98 |
| | | 58 | .404 | 4.974 | 127.790 | 1.00 | 40.93 |
| ATOM | 282 CE LYS A 35 | 57 | .410 | 3.827 | | | 44.56 |
| ATOM | 283 NZ LYS A 35. | | .754 | 2.656 | | | 44.56 |
| ATOM | 284 C LYS A 35 | | | | | | 55.10 |
| ATOM | | | .443 | 2.387 | 129.183 | 1.00 | 34.47 |
| | | 63 | .136 | 2.933 | 130.043 | 1 00 | 32.01 |
| MOTA | 286 N ASPA 36 | 62 | .180 | 1 086 | 129.190 | | 32.01 |
| ATOM | 287 CA ASP A 36 | | 710 | 0.233 | | | 36.28 |
| ATOM | 288 CB ASP A 36 | 62 | 145 | | | | 37.93 |
| ATOM | | 62. | .145 | -1.178 | 130.126 | 1.00 | 41.27 |
| | | | 731 | -2.117 | 131.157 | 1.00 | 43.77 |
| ATOM | 290 OD1 ASP A 36 | 62. | 660 | -1.793 | 132.360 | 1 00 | 43.92 |
| ATOM | 291 OD2 ASP A 36 | | 261 | -3 170 | 130.765 | | 43.92 |
| ATOM | 292 C ASP A 36 | | 227 | 0.176 | 130.703 | 1.00 | 45.78 |
| ATOM | | | | | 130.174 | 1.00 | 38.74 |
| ATOM | | | 902 | 0.187 | | 1.00 | 36.23 |
| | 294 N ALA A 37 | 64. | 760 | 0.127 | 128.958 | 1.00 | 37.96 |
| MOTA | 295 CA ALA A 37 | 66. | 201 | 0.080 | 128.768 | | |
| ATOM | 296 CB ALA A 37 | | | -0.000 | 127.299 | 1.00 | 39.49 |
| ATOM | 297 C ALA A 37 | | | -0.158 | 127.299 | 1.00 | 39.74 |
| ATOM | | | 832 | 1.386 | 129.244 | 1.00 | 40.09 |
| | | 67. | | 1:402 | 129.714 | 1.00 | 38 80 |
| ATOM | 299 N MET A 38 | 66. | 085 | 2.477 | 129.131 | 1.00 | 30.00 |
| ATOM | 300 CA MET A 38 | 66. | | 3 790 | 129.545 | 1.00 | 39.04 |
| ATOM | 301 CB MET A 38 | 65. | 066 | 4 069 | 129.545 | 1.00 | |
| ATOM | 200 | | | 4.863 | 128.640 | 1.00 | 36.66 |
| | | 66. | 335 | 4.744 | 127.173 | 1.00 | 39.16 |
| ATOM | 303 SD MET A 38 | 68. | 005 | 5.298 | 126.840 | | 37.55 |
| ATOM | 304 CE MET A 38 | 67. | 892 | | 127.287 | | |
| ATOM | 305 C MET A 38 | 66. | | | | 1.00 | 35.74 |
| ATOM | 306 O MET A 38 | | | | 130.995 | 1.00 | 40.58 |
| ATOM | | 66.4 | | 5.173 | 131.502 | 1.00 | 38.12 |
| | | 65.9 | 530 | 3.147 | 131.657 | 1.00 3 | 88.41 |
| ATOM | 308 CA ASN A 39 | 65.0 | 94 | | 133.039 | 1.00 | 12 46 |
| ATOM | 309 CB ASN A 39 | 66.2 | | | 133.979 | 1.00 | 42.40 |
| ATOM | 310 CG ASN A 39 | | | | | 1.00 4 | 16.06 |
| ATOM | | 67.1 | | 2 224 | 134.074 | 1.00 5 | 51.69 |
| | | 66.6 | | 2.175 | 134.487 | 1.00 5 | 4.33 |
| ATOM | 312 ND2 ASN A 39 | 68.3 | 96 | 2 313 | 133.695 | 1.00 4 | 0 13 |
| ATOM | 313 C ASN A 39 | 64.2 | | 4 594 | 133.134 | 1.00 4 | 2.13 |
| ATOM | 314 O ASN A 39 | 64.3 | | E 400 | 134 050 | 1.00 4 | 11.19 |
| ATOM | 315 N LEU A 40 | | | 3.402 | 134.050 | 1.00 4 | |
| ATOM | | 63.3 | | 4.746 | 132.188 | 1.00 4 | 0.22 |
| | | 62.4 | 27 | 5.909 | 132.170 | 1.00 3 | |
| ATOM | 317 CB LEU A 40 | 62.5 | 24 | 6 610 | 130.812 | 1 00 4 | 0.40 |
| ATOM | 318 CG LEU A 40 | 63.9 | 40 | 7 074 | 130.012 | 1.00 4 | 0.42 |
| ATOM · | 319 CD1 LEU A 40 | | | | 130.447 | 1.00 4 | 0.40 |
| ATOM | 330 CD3 1EG 2 40 | 63.9 | | | 129.088 | 1.00 3 | 2.75 |
| | 320 CD2 LEU A 40 | 64.4 | 70 | 8.031 1 | 131.513 | 1.00 3 | 8 89 |
| ATOM | 321 C LEU A 40 | 60.9 | | | 32.505 | | |
| ATOM | 322 O LEU A 40 | 60.0 | | | | 1.00 3 | |
| ATOM | 323 N ILE A 41 | 60.0 | | 6.409 1 | | 1.00 3 | |
| | | 60.7 | | 4.461 1 | | 1.00 3 | B.57 |
| ATOM | 324 CA ILE A 41 | 59.3 | 63 | 4.109 1 | .33.520 | 1.00 4 | 2.43 |
| Mota | 325 CB ILE A 41 | 58.5 | | 3.575 1 | | 1.00 3 | 0 17 |
| ATOM | 326 CG2 ILE A 41 | 59.1 | | | | 1.00 S | 13 |
| ATOM | 327 CG1 ILE A 41 | | - | 2.271 1 | | 1.00 3 | |
| | | 57.0 | | 3.367 1 | | 1.00 3 | 3.71 |
| MOTA | 328 CD1 ILE A 41 | 56.1 | | 2.920 1 | | 1.00 44 | |
| MOTA | 329 C ILE A 41 | 59.37 | | 3.056 1 | | 1.00 42 | |
| ATOM | 330 O ILE A 41 | 60.25 | 35 | | | | |
| | | 00.23 | 2 در | 2.195 1 | 24.054 | 1.00 43 | 1.05 |
| | | | | | | | |

| ATOM | 331 N ASP A 42 | 58.414 3.148 135.532 1 00 47 07 |
|--------|--------------------|--|
| ATOM | 332 CA ASP A 42 | 59 301 2 103 126 602 |
| ATOM | 333 CB ASP A 42 | 59 242 2 000 127 224 |
| MOTA | 334 CG ASP A 42 | ED 403 |
| MOTA | 335 OD1 ASP A 42 | 60 614 3 346 200 22.03 |
| ATOM | 336 OD2 ASP A 42 | 50 355 4 000 170 27.20 |
| ATOM | 337 C ASP A 42 | En an |
| MOTA | 338 O ASP A 42 | 1.00 31.22 |
| ATOM | 339 N GLU A 43 | ED #== |
| MOTA | 340 CA GLU A 43 | EE 045 |
| ATOM | 341 CB GLU A 43 | EC 22. |
| ATOM | 342 CG GLU A 43 | 56.234 -2.094 137.412 1.00 54.49 |
| ATOM | 343 CD GLU A 43 | 55.208 -3.178 137.185 1.00 60.55 55.524 -4.432 137.974 1.00 66 13 |
| ATOM | 344 OE1 GLU A 43 | 54 761 5 417 107 061 |
| ATOM | 345 - OE2 GLU A 43 | |
| ATOM | 346 C GLU A 43 | 56.536 -4.427 138.711 1.00 67.39 54.645 -0.178 137.178 1.00 50.30 |
| ATOM | 347 O GLU A 43 | 53 555 |
| ATOM | 348 N LYS A 44 | |
| ATOM | 349 CA LYS A 44 | 50 500 |
| ATOM | 350 CB LYS A 44 | |
| ATOM | 351 CG LYS A 44 | 54.013 2.004 140.112 1.00 54.73 |
| ATOM | 352 CD LYS A 44 | 53.190 3.229 140.542 1.00 58.07 |
| ATOM | 353 CE LYS A 44 | 53.705 4.500 139.853 1.00 61.24 |
| ATOM | 354 NZ LYS A 44 | 52.849 5.727 140.151 1.00 61.93 |
| ATOM | 355 C LYS A 44 | 51.501 5.644 139.519 1.00 62.80 |
| ATOM | 356 O. LYS A 44 | 52.929 2.387 137.875 1.00 44.52 |
| ATOM | 357 N GLU A 45 | 51.752 2.701 138.052 1.00 45.31 53.674 2.915 136 914 1.00 41.03 |
| ATOM | 358 CA GLU A 45 | E3 140 |
| ATOM | 359 CB GLU A 45 | 54 273 4 930 425 750 |
| MOTA | 360 CG GLU A 45 | EA 073 E 570 101 2:00 30:32 |
| ATOM | 361 CD GLU A 45 | 56 241 6 222 11.00 40.30 |
| ATOM | 362 OE1 GLU A 45 | |
| ATOM | 363 OE2 GLU A 45 | EC 306 |
| ATOM | 364 C GLU A 45. | 52 470 |
| ATOM . | 365 O GLU A 45 | 51 702 2 007 404 |
| ATOM | 366 N LEUA 46 | E3 700 |
| MOTA | 367 CA LEU A 46 | 52 365 1 202 203 203 |
| ATOM | 368 CB LEU A 46 | 53.222 0.219 133.034 1.00 35.52 |
| ATOM | 369 CG LEU A 46 | 52.873 -0.619 131.811 1.00 43.75 |
| ATOM | 370 CD1 LEU A 46 | 52.571 0.292 130.630 1.00 42.06 |
| ATOM | 371 CD2 LEU A 46 | 54.035 -1.544 131.500 1.00 42.90 |
| MOTA | 372 C LEU A 46 | 50.852 0.467 133.780 1.00 40.03 |
| ATOM | 373 O LEUA 46 | 50.741 -0.306 134.730 1.00 39.37 |
| ATOM | 374 N ILE A 47 | 49.861 0.718 132.928 1.00 34.03 |
| MOTA | 375 CA ILE A 47 | 48.560 0.068 133.033 1.00 32.12 |
| ATOM | 376 CB ILE A 47 | 47.413 1.087 132.937 1.00 32.35 |
| ATOM | 377 CG2 ILE A 47 | 46.069 0.360 132.833 1.00 30.60 |
| Arom | 378 CG1 ILE A 47 | 47.448 2.015 134.156 1.00 36.56 |
| MOTA | 379 CD1 ILE A 47 | 46.372 3.080 134.162 1.00 35 46 |
| MOTA | 380 C ILE A 47 | 48.428 ~0.920 131.882 1.00 33.67 |
| ATOM | 381 O ILE A 47 | 48.505 -0.532 130.717 1.00 27.64 |
| MOTA | 382 N LYS A 48 | 48.231 -2.195 132.205 1.00 32.98 |
| MOTA | 383 CA LYS A 48 | 48.102 -3.224 131.176 1.00 30.98 |
| MOTA | 384 CB LYS A 48 | 48.038 -4.609 131.821 1.00 39.21 |
| MOTA | 385 CG LYS A 48 | 47.956 -5.747 130.819 1.00 46.81 |
| TOM | 386 CD LYS A 48 | 47.989 -7.102 131.509 1.00 50.75 |
| TOM | 387 CE LYS A 48 | 47.967 -8.240 130.492 1.00 54.43 |
| MOTA | 388 NZ LYS A 48 | 49.151 -8.199 129.580 1.00 50.43 |
| MOTA | 389 C LYS A 48 | 46.869 -3.006 130.310 1.00 29.55 |
| TCM | 390 C LYS A 48 | 45.764 -2.840 130.820 1.00 29.65 |
| TOM | 391 N SER A 49 | 47.071 -2.992 128.996 1.00 30.69 |
| MOT | 392 CA SER A 49 | 45.989 -2.802 128.033 1.00 29.32 |
| MOT | 393 CB SER A 49 | 46.551 -2.805 126.609 1.00 31.53 |
| MOT | 394 OG SER A 49 | 47.571 -1.834 126.443 1.00 30.74 |
| TOM | 395 C SER A 49 | 44.952 -3.916 128.147 1.00 31.31 |
| TOM | 396 O SER A 49 | 45.295 -5.059 128.436 1.00 34.44 |
| | | • |

| ATOM | 397 N ARG A 50 | 43.688 -3.582 127.922 1.00 32.87 |
|------|--------------------------------------|--|
| MOTA | 398 CA ABG A 50 | 40 600 4 600 |
| MOTA | 399 CB ARG A 50 | 41 616 4 100 4 |
| ATOM | 400 CG ARG A 50 | |
| ATOM | 401 CD ARG A 50 | |
| ATOM | 402 NE ARG A 50 | 1.00 30.40 |
| ATOM | 403 CZ ARG A 50 | |
| ATOM | 404 NH1 ARG A 50 | |
| ATOM | 405 NH2 ARG A 50 | |
| ATOM | 406 C ARG A 50 | 2.00 24.52 |
| ATOM | 407 O ARG A 50 | |
| ATOM | 408 N PRO A 51 | 1.00 24.02 |
| ATOM | 409 CD PRO A 51 | |
| MOTA | 410 CA PRO A 51 | |
| ATOM | 411 CB PRO A 51 | 1.00 30.36 |
| ATOM | 412 CG PRO A 51 | |
| ATOM | 413 C PRO A 51 | |
| ATOM | 414 O PRO A 51 | |
| ATOM | 415 N ALA A 52 | 1.00 25.04 |
| ATOM | 416 CA ALA A 52 | |
| ATOM | 417 CB ALA A 52 | |
| ATOM | 418 C ALA A 52 | 37.365 -2.447 122.956 1.00 28.67 36.437 -4.321 124.288 1.00 32.39 |
| ATOM | 419 O ALA A 52 | |
| ATOM | 420 N THR A 53 | |
| ATOM | 421 CA THR A 53 | |
| ATOM | 422 CB THR A 53 | |
| MOTA | 423 OG1 THR A 53 | |
| ATOM | 424 CG2 THR A 53 | 32.734 -3.193 125.970 1.00 29.52 33.998 -4.579 127.493 1.00 36.45 |
| ATOM | 425 C THR A 53 | 33.411 -4.700 123.702 1.00 38.94 |
| ATOM | 426 O THR A 53 | 33.559 -3.689 123.012 1.00 32.67 |
| ATOM | 427 N LYS A 54 | 32.577 -5.679 123.372 1.00 39.19 |
| ATOM | 428 CA LYS A 54 | 31.792 -5.595 122.152 1.00 40.71 |
| MOTA | 429 CB LYS A 54 | 30.933 -6.851 121.994 1.00 41.68 |
| MOTA | 430 CG LYS A 54 | 30.367 -7.034 120.597 1.00 49.42 |
| ATOM | 431 CD LYS A 54 | 29.541 -8.310 120.508 1.00 51.82 |
| ATOM | 432 CE LYS A 54 | 29.075 -8.588 119.087 1.00 52.94 |
| MOTA | 433 NZ LYS A 54 | 30.216 -8.879 118.182 1.00 54.26 |
| ATOM | 434 C LYS A 54 | 30.913 -4.347 122.237 1.00 39.46 |
| ATOM | 435 O LYS A 54 | 30.719 -3.637 121.249 1.00 37.19 |
| ATOM | 436 N GLUA 55 | 30.404 -4.075 123.434 1.00 36.71 |
| MOTA | 437 CA GLU A 55 | 29.554 -2.913 123.665 1.00 36.18 |
| ATOM | 438 CB GLU A 55 | 29.109 -2.877 125.127 1.00 42.16 |
| MOTA | 439 CG GLU A 55 | 28.223 -1.694 125.476 1.00 46.04 |
| ATOM | 440 CD GLU A 55 | 27.873 -1.639 126.953 1.00 51.15 |
| ATOM | 441 OE1 GLU A 55 | 27.092 -0.748 127.343 1.00 56.53 |
| ATOM | 442 OE2 GLU A 55 443 C GLU A 55 | 28.382 -2.482 127.727 1.00 51.67 |
| ATOM | | 30.278 -1.607 123.32: 1.00 35.45 |
| MOTA | | 29.721 -0.729 122.66 1.00 29.11 |
| MOTA | | 31.518 -1.476 123.776 1.00 27.82 |
| ATOM | | 32.289 -0.269 123.497 1.00 34.70 |
| ATOM | | 33.635 -0.329 124.232 1.00 30.71 |
| MOTA | 448 CG GLU A 56 449 CD GLU A 56 | 33.474 -0.484 125.746 1.00 35.09 |
| MOTA | | 34.787 -0.675 126.479 1.00 32.29 |
| ATOM | . = - | 35.645 -1.434 125.986 1.00 34.54 |
| ATOM | | 34.951 -0.094 127.569 1.00 33.25 |
| ATOM | | 32 495 -0.104 121.988 1.00 32.51 |
| ATOM | 453 O GLUA 56 454 N LEUA 57 | 32.341 0.990 121.444 1.00 29.59 |
| ATOM | | 32.827 -1.196 121.311 1.00 35.58 |
| ATOM | 455 CA LEU A 57 456 CB LEU A 57 | 33.039 -1.147 119.871 1.00 35.70 |
| ATOM | 450 CB LEU A 57 | 33.475 -2.512 119.334 1.00 35.25 |
| ATOM | 457 CG LEU A 57 | 34.829 -3.030 119.814 1.00 36.19 |
| ATOM | 450 CD1 LEU A 57 459 CD2 LEU A 57 | 35.095 -4.390 119.183 1.00 33.69 |
| ATOM | 460 C LEU A 57 | 35.925 -2.041 119.433 1.00 32.61 |
| ATOM | 461 O LEU A 57 | 31.772 -0.717 119.157 1.00 36.02 |
| ATOM | 462 N LEU A 58 | 31.828 0.067 118.205 1.00 32.72 |
| ATCM | and M mo w no | 30.631 -1.228 119.620 1.00 32.35 |

| ATOI | M 463 CA LEU A 58 | 20 353 0 000 454 |
|------|--------------------|----------------------------------|
| ATO | 4 464 65 55 | 29.353 -0.898 119.004 1.00 33.21 |
| ATO | A ACC TO DOUGH JO | 28.260 -1.844 119.495 1.00 35.17 |
| | 45 250 Y 36 | 28.504 -3.296 119.077 1.00 33.71 |
| MOTA | DLU A 38 | |
| ATOM | 467 CD2 LEU A 58 | 20 20 20 20 20 30.80 |
| ATOM | | 20 210 22,13,0 1.00 38.30 |
| ATOM | | 28.940 0.543 119.222 1.00 30 99 |
| | | 27.915 0.985 118.700 1.00 35.50 |
| ATOM | | 20 722 |
| ATOM | 471 CA LEU A 59 | |
| ATOM | . 450 | 1.00 30.3/ |
| ATOM | | 30.38/ 3.279 121.268 1.00 28.01 |
| | HAU R. J. | 30.174 2.828 122.716 1.00 32.19 |
| ATOM | | 31 340 32.13 |
| ATOM | 475 CD2 LEU A 59 | 20 24.83 |
| ATOM | 476 C LEU A 59 | 20.152 1.00 25.65 |
| ATOM | 477 6 | 29.632 3.405 118.890 1.00 31.26 |
| | - 220 % | 29.020 4.442 118.652 1.00 31.80 |
| MOTA | | |
| ATOM | 479 CA PHE A 60 | 1.00 23.79 |
| ATOM | 480 CB PHE A 60 | |
| ATOM | | 32.131 4.055 116.637 1.00 29.99 |
| | | 32.443 4.691 115.299 1.00 28.88 |
| ATOM | 482 CD1 PHE A 60 | 71 700 5 700 |
| ATOM | 483 CD2 PHE A 60 | |
| ATOM | 484 CE1 PHE A 60 | |
| ATOM | 485 CE2 PHE A 60 | 31.959 6.351 113.592 1.00 26.12 |
| | | 33.709 4.740 113.226 1.00 25.98 |
| ATOM | 486 CZ PHE A 60 | 32.963 5.828 112.781 1.00 24.53 |
| ATOM | 487 C PHE A 60 | |
| ATOM | 488 O PHE A 60 | 20 010 2 054 444 555 |
| ATOM | | |
| MOTA | 400 | 31.195 1.363 115.543 1.00 32.85 |
| | 404 | 31.075 0.418 114.431 1.00 34.59 |
| ATOM | 491 CB HIS A 61 | 70 707 0 400 400 - |
| ATOM | 492 CG HIS A 61 | 77 576 6 655 444 |
| ATOM | 493 CD2 HIS A 61 | 34 335 |
| ATOM | 404 | 24 200 |
| ATOM | | 34.328 0.786 115.133 1.00 37.78 |
| | | 35.390 1.382 114.619 1.00 37.50 |
| ATOM | 496 NE2 HIS A 61 | 26 260 1 242 442 444 |
| ATOM | 497 C HIS A 61 | 20 024 |
| ATOM | 498 O HIS A 61 | 70 717 0 610 115 |
| MOTA | 499 N THR A 62 | |
| ATOM | | 29.462 -1.015 113.327 1.00 39.73 |
| | F.0.1 | 28.278 -1.868 113.218 1.00 38.05 |
| MOTA | 501 CB THR A 62 | 27.682 -1.825 111.804 1.00 37.22 |
| ATOM | 502 OG1 THR A 62 | |
| MOTA | 503 CG2 THR A 62 | 27 340 0 404 |
| ATOM | 504 C THR A 62 | |
| ATOM | CAC . | 28.598 -3.317 113.551 1.00 39.06 |
| | | 29.731 -3.768 113.392 1.00 39 32 |
| ATOM | 506 N GLUA 63 | 27.582 -4.034 114.017 1.00 40.92 |
| ATOM | 507 CA GLU A 63 | 77 606 5 445 |
| MOTA | 508 CB GLU A 63 | 26 202 |
| ATOM | 509 CG GLU A 63 | 26 260 |
| ATOM | | 26.269 -7.451 115.171 1.00 46.90 |
| | | 26.472 -7.593 116.665 1.00 53.11 |
| MOTA | 511 OE1 GLU A 63 | 26.601 -8.739 117.152 1.00 52.78 |
| ATOM | 512 OE2 GLU A 63 | |
| MOTA | 513 C GLUA 63 | 20 200 |
| ATOM | 514 O GLU A 63 | |
| ATOM | | 29.272 -7.011 113.481 1.00 29.70 |
| | | 27.755 -6.119 112.074 1.00 35.85 |
| atom | 516 CA ASP A 64 | 28.198 -6.841 110.886 1.00 37.61 |
| ATOM | 517 CB ASP A 64 | 27.363 -6.382 109.697 1.00 43.30 |
| ATOM | 518 CG ASP A 64 | |
| ATOM | 519 OD1 ASP A 64 | |
| ATOM | 520 OD2 ASP A 64 | 28.290 -4.269 109.089 1.00 52.15 |
| | | 26.298 -4.285 110.018 1.00 53.97 |
| ATOM | 521 C ASP A 64 | 29.673 -6.660 110.594 1.00 35.04 |
| ATOM | 522 O ASP A 64 | 30.379 -7.625 110.303 1.00 33.60 |
| ATOM | 523 N TYR A 65 | |
| ATOM | 524 CA TYR A 65 | |
| | | 31.554 -5.153 110.419 1.00 32.91 |
| ATOM | 525 CB TYR A 65 | 31.793 -3.637 110.375 1.00 34.80 |
| ATOM | 526 CG TYR A 65 | 33.247 -3.253 110.219 1.00 35 19 |
| ATOM | 527 CD1 TYR A 65 | 34.009 -3.751 109.163 1.00 28.43 |
| ATOM | 528 CE1 TYR A 65 | 75 7- |
| | | 35.352 -3.411 109.024 1.00 32.52 |

| | | | | | • | |
|------|-------|-------|---------|----------|--|----------|
| MOTA | 529 | CI CI | OZ TYR | A 65 | 33.863 -2.398 111.134 1.0 | 00 34.08 |
| MOTA | 530 |) CI | E2 TYR | A 65 | | 0 29.89 |
| ATOM | 531 | L C2 | TYR | A 65 | | 0 35.29 |
| MOTA | 532 | OF | I TYR | A 65 | | 0 29.81 |
| ATOM | 533 | 3 C | TYR | A 65 | | 0 27.65 |
| ATOM | 534 | 1 0 | TYR | | | 0 27.65 |
| ATOM | 535 | N | ILE . | | | 0 27.32 |
| ATOM | 536 | CA | | | | 0 25.82 |
| ATOM | 537 | | | | | 0 32.25 |
| ATOM | 538 | | 2-ILE | | | 0 28.85 |
| ATOM | 539 | | 1 ILE | | | |
| ATOM | 540 | | 1 ILE | | | 0 31.48 |
| MOTA | 541 | | ILE 2 | | · | 0 38.02 |
| ATOM | 542 | | ILE | | | 0 31.21 |
| ATOM | 543 | | ASN 2 | | | 0 30.25 |
| ATOM | 544 | | | | | 0 33.28 |
| ATOM | 545 | | | | 30 | 0 35.87 |
| ATOM | 546 | | | | | 0 33.07 |
| ATOM | 547 | | 1 ASN A | | | 0 37.34 |
| ATOM | 548 | ND: | | | | 0 35.20 |
| ATOM | 549 | C | ASN A | | | 0 34.83 |
| ATOM | 550 | ō | ASN A | | 32.499 -10.198 112.219 1.0 | 0 31.00 |
| ATOM | 551 | N | THR A | | | 0 37.26 |
| ATOM | 552 | CA | THR A | | | 0 30.91 |
| ATOM | 553 | CB | THR A | | | 0 31.04 |
| ATOM | 554 | | I THR A | | | 0 34.01 |
| ATOM | 555 | CG2 | | | 31.780 -9.037 108.352 1.0 | 0 33.26 |
| ATOM | 556 | C | THR A | | | 0 30 84 |
| ATOM | 557 | ō | THR A | | | 0 33.31 |
| ATOM | 558 | Ŋ | LEU A | | | 32.52 |
| ATOM | 559 | CA | LEU A | | 35.267 -8.768 111.117 1.00 36.669 -8.686 111.534 1.00 | 30.30 |
| ATOM | 560 | CB | LEU A | | | 28.20 |
| ATOM | 561 | CG | LEU A | - | 36.938 -7.409 112.351 1.00 | 28.25 |
| ATOM | 562 | | LEU A | | | 30.18 |
| ATOM | 563 | | LEU A | | | 31.08 |
| ATOM | 564 | C | LEU A | 69 | | 27.85 |
| ATOM | 565 | õ | LEU A | 69 | | 31.65 |
| ATOM | 566 | N | MET A | 70 | | 23.95 |
| ATOM | 567 | CA | MET A | 70 | | 30.78 |
| ATOM | . 568 | CB | MET A | 70 | 36.411 -11.383 114.193 1.00 | 34.50 |
| ATOM | 569 | CG | MET A | 70 | 35.318 -11.486 115.258 1.00 35.203 -10.259 116.147 1.00 | |
| ATOM | 570 | SD | MET A | 70 | | 36.26 |
| ATOM | 571 | CE | MET A | 70 | | 37.52 |
| ATOM | 572 | C | MET A | 70 | 34.633 -11.815 118.403 1.00 | 37.36 |
| ATOM | 573 | 0 | MET A | 70 | | 33.33 |
| ATOM | 574 | N | GLU A | 71 | | 31.47 |
| ATOM | 575 | CA | GLU A | 71 | | 35.37 |
| ATOM | 576 | CB | GLU A | 71 | | 36.6 |
| ATOM | 577 | CG | GLU A | 71 | 34.245 -14.160 110.834 1.00 | 37.3 |
| ATOM | 578 | CD | GLU A | 71 | 34.206 -15.359 109.897 1.00 | 46.37 |
| ATOM | 579 | | GLU A | 71 | 34.257 -16.693 110.633 1.00 | 46.37 |
| | | | GLU A | 71 | | 48.94 |
| ATOM | 580 | | | 71 | 34.190 -16.705 111.882 1.00 | 45.53 |
| MOTA | 581 | C | GLU A | | 36.732 -14.169 110.769 1.00 | 35.96 |
| MOTA | 582 | 0 | GLU A | 71 | 37.342 -15.228 110.617 1.00 | 32.99 |
| ATOM | 583 | N | ALA A | 72 | 37.079 -13.039 110.159 1.00 | 36.50 |
| MOTA | 584 | CA | ALA A | 72 | 38.225 -12.981 109.264 1.00 | 33.98 |
| ATOM | 585 | CB | ALA A | 72 | 38.366 -11.580 108.675 1.00 | 33.23 |
| ATOM | 586 | C | ALA A | 72 | 39.498 -13.362 109.998 1.00 | 34.60 |
| ATOM | 587 | 0 | ALA A | 72 73 | | 31.53 |
| ATOM | 588 | N | GLU A | 73 | 39.647 -12.873 11224 1.00 | 30.87 |
| ATOM | 589 | CA | GLU A | 73 | | 29.66 |
| ATOM | 590 | CB | GLU A | 73 | | 33.33 |
| ATOM | 591 | CG | GLU A | 73 | | 32.80 |
| ATOM | 592 | CD | GLU A | 73 | | 40.07 |
| ATOM | 593 | | GLU A | 73 | | 41.02 |
| MOTA | 594 | OE2 | GLU A | 73 | 42.298 -12.138 116.372 1.00 | 41.21 |

| MOTA | 595 | С | GLU A | 73 | 40.906 -14.615 112.485 1.00 31.73 |
|-------|-----------------|-----|-------|------|-----------------------------------|
| ATOM | 596 | Ō | GLU A | 73 | 41.957 -15.249 112.409 1.00 32.96 |
| | | | - | | |
| MOTA | 597 | N | ARG A | 74 | 39.798 -15.145 112.992 1.00 35.85 |
| ATOM | 598 | CA | ARG A | 74 | 39.847 -16.511 113.502 1.00 43.24 |
| MOTA | 599 | CB | ARG A | 74 | 38.548 -16.892 114.216 1.00 43.63 |
| | 600 | CG | ARG A | 74 | 37.450 -17.349 113.294 1.00 51.20 |
| ATOM | | | | | |
| MOTA | 601 | CD | ARG A | 74 | 36.366 -18.087 114.063 1.00 51.13 |
| ATOM | 602 | NE | ARG A | 74 | 35.534 -18.871 113.158 1.00 57.40 |
| ATOM | 603 | CZ | ARG A | .74 | 35.991 -19.870 112.403 1.00 56.36 |
| | | | | 74 | 37.273 -20.208 112.446 1.00 51.10 |
| ATOM | 604 | NH1 | | | |
| ATOM | 605 | NH2 | ARG A | 74 | 35.172 -20.517 111.586 1.00 58.75 |
| MOTA | 606 | С | ARG A | 74 | 40.125 -17.506 112.372 1.00 43.06 |
| | 607 | ō | ARG A | 74 | 40.916 -18.429 112.541 1.00 42.52 |
| ATOM | | | | | |
| MOTA | 608 | N | SER A | 75 | 39.485 -17.305 111.222 1.00 43.63 |
| ATOM | 609 | CA | SER A | 75 | 39.670 -18.186 110.066 1.00 44.93 |
| MOTA | 610 | CB | SER A | 75 | 38.485 -18.089 109.113 1.00 42.05 |
| | 611 | OG | SER A | 75 | 38.420 -16.799 108.532 1.00 38.43 |
| ATOM | | | | | |
| MOTA | 612 | С | SER A | 75 | 40.910 -17.797 109.282 1.00 46.44 |
| ATOM | 613 | 0 | SER A | 75 | 41.339 -18.522 108.383 1.00 45.17 |
| ATOM | 614 | N | GLN A | 76 | 41.466 -16.638 109.618 1.00 46.18 |
| | 615 | CA | GLN A | 76 | 42.642 -16.116 108.936 1.00 44.73 |
| MOTA | | | | | |
| ATOM | 616 | CB | GLN A | 76 | 43.868 -16.973 109.226 1.00 37.36 |
| MOTA | 617 | CG | GLN A | 76 | 45.162 -16.208 109.045 1.00 43.96 |
| ATOM | 618 | CD | GLN A | 76 | 45.415 -15.214 110.176 1.00 41.86 |
| | 619 | OE1 | | 76 | 44.499 -14.537 110.655 1.00 37.78 |
| ATOM | | | | | |
| ATOM | 620 | NE2 | | 76 | 46.669 -15.111 110.591 1.00 45.00 |
| MOTA | 621 | С | GLN A | 76 | 42.374 -16.120 107.429 1.00 44.17 |
| MOTA | 622 | 0 | GLN A | 76 | 43.233 -16.495 106.630 1.00 40.49 |
| ATOM | 623 | N | SER A | . 77 | 41.168 -15.713 107.053 1.00 43.11 |
| | | | | | 40.784 -15.667 105.649 1.00 44.66 |
| MOTA | 624 | CA | SER A | 77 | |
| ATOM | 625 | CB | SER A | 77 | 40.182 -17.004 105.220 1.00 44.56 |
| ATOM | 626 | OG | SER A | 77 | 38.974 -17.246 105.925 1.00 42.58 |
| ATOM | 627 | С | SER A | 77 | 39.747 -14.573 105.448 1.00 44.80 |
| | 628 | ō | SER A | 77 | 39.096 -14.142 106.395 1.00 45.11 |
| ATOM | | | | | |
| MOTA | 629 | N | VAL A | 78 | 39.590 -14.137 104.207 1.00 46.06 |
| MOTA | 630 | CA | VAL A | 78 | 38.632 -13.095 103.888 1.00 47.65 |
| ATOM | 631 | CB | VAL A | 78 | 39.107 -12.245 102.701 1.00 49.63 |
| ATOM | 632 | | VAL A | 78 | 38.076 -11.167 102.391 1.00 51.25 |
| | | | | 78 | 40.454 -11.627 103.017 1.00 53.00 |
| ATOM | 633 | | VAL A | | |
| ATOM' | 634 | С | VAL A | 78 | 37.275 -13.682 103.530 1.00 48.07 |
| MOTA | 635 | 0 | VAL A | 78 | 37.111 -14.301 102.480 1.00 42.31 |
| ATOM | 636 | N | PRO A | 79 | 36.282 -13.492 104.407 1.00 49.82 |
| | | CD | PRO A | 79 | 36.347 -12.782 105.696 1.00 50.81 |
| ATOM | 637 | | | | |
| ATOM | 638 | CA | PRO A | 79 | 34.927 -13.998 104.186 1.00 51.31 |
| ATOM | 639 | CB | PRO A | 79 | 34.170 -13.450 105.396 1.00 53.13 |
| MOTA | 640 | CG | PRO A | ~9 | 35.244 -13.469 106.469 1.00 53.50 |
| | 641 | C | PRO A | :9 | 34.343 -13.517 102.858 1.00 52.42 |
| MOTA | | | | | |
| ATOM | 642 | 0 | PRO A | ∵9 | |
| ATOM | 643 | N | LYS A | 80 | 33.482 -14.343 102.273 1.00 49.63 |
| MOTA | 644 | CA | LYS A | 80 | 32.824 -14.053 101.002 1.00 51.62 |
| | 645 | CB | LYS A | 80 | 31.632 -15.004 100.822 1.00 53.92 |
| MOTA | | | | | 30.817 -14.808 99.545 1.00 56.27 |
| ATOM | 646 | CG | LYS A | 80 | |
| MOTA | 647 | CD | LYS A | 80 | 29.586 -15.712 99.560 1.00 56.61 |
| MOTA | 648 | CE | LYS A | 80 | 28.744 -15.579 98.298 1.00 56.04 |
| | 649 | NZ | LYS A | 80 | 29.471 -16.036 97.081 1.00 58.90 |
| ATOM | | | | | |
| ATOM | 650 | C | LYS A | 80 | |
| MOTA | 6 51 | 0 | LYS A | 80 | 31.539 -12.140 101.689 1.00 49.22 |
| ATOM | 652 | N | GLY A | 81 | 32.821 -11.914 99.842 1.00 51.14 |
| | 653 | CA | GLY A | 81 | 32.418 -10.537 99.592 1.00 47.07 |
| ATOM | | | | | |
| ATOM | 654 | С | GLY A | 81 | |
| ATOM | 655 | 0 | GLY A | 81 | 32.671 -8.301 100.397 1.00 43.90 |
| ATOM | 656 | N | ALA A | 82 | 33.504 -9.942 101.681 1.00 44.50 |
| | 657 | CA | ALA A | 82 | 33.973 -9.029 102.715 1.00 44.69 |
| ATOM | | | | 82 | 34.497 -9.825 103.903 1.00 44.62 |
| ATOM | 658 | CB | ALA A | | |
| ATOM | 659 | С | ALA A | 82 | 35.049 -8.073 102.215 1.00 41.82 |
| ATOM | 660 | 0 | ALA A | 82 | 35.132 -6.925 102.662 1.00 35.92 |
| | | - | | | • |

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Figure 18-11

| MOTA | 661 N ARG A 83 | 35.874 -8.549 101 289 1 00 42 20 |
|------|------------------|--|
| ATOM | 662 CA ARG A 83 | 36 959 7 742 100 743 |
| ATOM | 663 CB ARG A 83 | 37 71E 0 mm |
| ATOM | 664 CG ARG A 83 | 30 000 7 007 1.00 40.00 |
| ATOM | 665 CD ARG A 83 | 30.222 1.00 51.32 |
| ATOM | 666 NE ARG A 83 | 39.636 -8.632 98.086 1.00 55.55 |
| ATOM | 5.50 | 40.995 -8.164 97.810 1.00 64.08 |
| ATOM | | 41.330 -6.905 97.540 1.00 63 01 |
| ATOM | | 40.403 -5.954 97.504 1.00 62.76 |
| | 669 NH2 ARG A 83 | 42.599 -6.600 97.304 1.00 59 66 |
| ATOM | 670 C ARG A 83 | 36.453 -6.435 100.134 1 00 44 50 |
| ATOM | 671 O ARG A 83 | 37.002 -5.365 100.395 1.00 38.05 |
| ATOM | 672 N GLUA 84 | 35.404 -6.528 99.323 1.00 41.82 |
| MOTA | 673 CA GLUA 84 | 34.824 -5.356 98.678 1.00 41.44 |
| MOTA | 674 CB GLUA 84 | 34.145 -5.765 97.367 1.00 46.27 |
| ATOM | 675 CG GLU A 84 | 22 22 20 20.27 |
| MOTA | 676 CD GLUA 84 | 24 2.01 |
| MOTA | 677 OE1 GLU A 84 | 24 27.300 1.00 34.12 |
| MOTA | 678 OE2 GLU A 84 | 7, 04 1.00 33.08 |
| MOTA | 679 C GLU A 84 | 22 024 |
| ATOM | 680 O GLU A 84 | 22 500 37.36 |
| MOTA | 681 N LYS A 85 | 33 130 5 301 100 34.30 |
| ATOM | 682 CA LYS A 85 | 100 30.00 |
| ATOM | 683 CB LYS A 85 | 1.00 36.95 |
| ATOM | 684 CG LYS A 85 | 20 200 200 200 200 200 200 200 200 200 |
| ATOM | 685 CD LYS A 85 | 20 110 40.72 |
| ATOM | 686 CE LYS A 85 | 20 40.21 |
| ATOM | 687 NZ LYS A 85 | 25.00 |
| ATOM | 688 C LYS A 85 | 26.859 -6.513 104.287 1.00 52.72 |
| ATOM | 689 O LYS A 85 | 32.785 -4.008 102.513 1.00 36.48 |
| ATOM | 690 N TYR A 86 | 32.353 -2.949 102.966 1.00 32.97 |
| ATOM | 691 CA TYR A 86 | 33.819 -4.649 103.041 1.00 33.69 |
| ATOM | | 34.468 -4.169 104.250 1.00 35.23 |
| ATOM | C00 | 34.410 -5.281 105.300 1.00 33.65 |
| ATOM | 604 | 32.990 -5.665 105.680 1.00 35.09 |
| ATOM | COC | 32.165 -4.765 106.351 1.00 34.06 |
| ATOM | 505 | 30.866 -5.100 106.704 1.00 34.32 |
| ATOM | COR | 32.4/0 -6.923 105.365 1.00 33.17 |
| MOTA | COO | 31.162 -7.271 105.716 1.00 33.91 |
| ATOM | | 30.369 -6.350 106.386 1.00 34.21 |
| ATOM | | 29.079 -6.658 106.738 1.00 35.20 |
| ATOM | = | 35.901 -3.672 104.046 1.00 36.09 |
| ATOM | 700 | 36.552 -3.208 104.984 1.00 36.06 |
| ATOM | | 36.382 -3.777 102.814 1.00 36.46 |
| ATOM | 704 | 37.712 -3.313 102.441 1.00 32.71 |
| ATOM | 705 | 37.768 -1.791 102.576 1.00 36.26 |
| ATOM | 704 | 38.989 -1.199 101.926 1.00 37.25 |
| ATOM | 700 | 39.305 -1.518 100.784 1.00 36.29 |
| ATOM | | 39.675 -0.320 102.640 1.00 45.25 |
| ATOM | 700 | 38.855 -3.956 103.217 1.00 34.73 |
| | | 39.868 -3.315 103.512 1.00 33.23 |
| ATOM | 710 N ILE A 88 | 38.687 -5.237 103.523 1.00 32.48 |
| MOTA | 711 CA ILE A 88 | 39.676 -6.018 104.248 1.00 33.65 |
| ATOM | 712 CB ILE A 88 | 39.030 -6.732 105.445 1.00 38.66 |
| ATOM | 713 CG2 ILE A 88 | 40.021 -7.680 106.081 1.00 41.31 |
| ATOM | 714 CG1 ILE A 88 | 38.536 -5.707 106.461 1.00 40.45 |
| ATOM | 715 CD1 ILE A 88 | 39.641 -4.953 107.124 1.00 42.25 |
| ATOM | 716 C ILE A 88 | 40.251 -7.090 103.318 1.00 37.36 |
| MOTA | 717 O ILE A 88 | 39.555 -7.587 102.431 1.00 35.47 |
| MOTA | 718 N GLY A 89 | 41.517 -7.446 103.520 1.00 31.52 |
| ATOM | 719 CA GLY A: 89 | 42.124 -8.477 102.698 1.00 33.53 |
| MOTA | 720 C GLY A 89 | 43.134 -7.994 101.675 1.00 34.50 |
| MOTA | 721 O GLY A 89 | 43.951 -8.777 101.186 1.00 32.81 |
| ATOM | 722 N GLY A 90 | 43.071 -6.710 101.335 1.00 31.39 |
| ATOM | 723 CA GLY A 90 | 44.005 -6.158 100.371 1.00 23.90 |
| ATOM | 724 C GLY A 90 | 45.340 -5.893 101.040 1.00 28.78 |
| ATOM | 725 O GLY A 90 | 45.563 -6.339 102.163 1.00 21.71 |
| MOTA | 726 N TYR A 91 | 46.221 -5.155 100.367 1.00 28.26 |
| | • | , 3.123 2-0.007 1.00 28.26 |
| | | |

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Figure 18-12

| MOTA | 727 CA TYR A 91 | 47.539 -4.850 100.918 1.00 27.34 |
|--------------|------------------------------------|--|
| MOTA | 728 CB TYR A 91 | 10 177 1 265 00 000 |
| MOTA | 729 CG TYR A 91 | 40 000 |
| MOTA | 730 CD1 TYR A 91 | 40 774 1 000 |
| MOTA | 731 CE1 TYR A 91 | 47 070 0 000 00 000 |
| MOTA | 732 CD2 TYR A 91 | 47 341 2 002 00 24,09 |
| MOTA | 733 CE2 TYR A 91 | 16 031 |
| MOTA | 734 CZ TYR A 91 | |
| MOTA | 735 OH TYR A 91 | 2.00 23.04 |
| ATOM | 736 C TYR A 91 | 27.020 1.00 29.01 |
| ATOM | 737 O TYR A 91 | |
| ATOM | 738 N GLUA 92 | 1.00 27.20 |
| MOTA | 739 CA, GLU A 92 | |
| MOTA | 740 CB GLU A 92 | 45 00 ZB.50 |
| ATOM | 741 CG GLU A 92 | 15 200 20,57 |
| MOTA | 742 CD GLU A 92 | 1.00 30.34 |
| ATOM | 743 OE1 GLU A 92 | 1.00 37.40 |
| ATOM | 744 OE2 GLU A 92 | 44 505 |
| ATOM | 745 C GLU A 92 | |
| MOTA | 746 O GLUA 92 | |
| ATOM | 747 N . ASN A 93 | 1.00 24.00 |
| MOTA | 748 CA ASN A 93 | 1.00 20.51 |
| ATOM | 749 CB ASN A 93 | 10 707 |
| MOTA | 750 CG ASN A 93 | 1.00 24.31 |
| ATOM | 751 OD1 ASN A 93 | 42.738 -1.488 105.405 1.00 28.61 43.428 -0.727 106.079 1.00 25.30 |
| MOTA | 752 ND2 ASN A 93 | 41.987 -1.063 104.393 1.00 20.45 |
| ATOM | 753 C ASN A 93 | 43.999 -5.132 105.407 1.00 24.79 |
| ATOM | 754 O ASNA 93 | 42.905 -5.680 105.291 1.00 21.89 |
| ATOM | 755 N PRO A 94 | 45.142 -5.828 105.429 1.00 24.60 |
| MOTA | 756 CD PRO A 94 | 46.493 -5.246 105.540 1.00 22.93 |
| MOTA | 757 CA PRO A 94 | 45.241 -7.285 105.312 1.00 27.23 |
| ATOM | 758 CB PRO A 94 | 46.730 -7.488 105.093 1.00 25.46 |
| ATOM | 759 CG PRO A 94 | 47.299 -6.431 106.046 1.00 26.20 |
| ATOM | 760 C PRO A 94 | 44.743 -8.112 106.489 1.00 31.04 |
| MOTA | 761 O PRO A 94 | 44.411 -7.589 107.558 1.00 29.10 |
| MOTA | 762 N VAL A 95 | 44.696 -9.422 106.266 1.00 28.27 |
| ATOM | 763 CA VAL A 95 | 44.299 -10.367 107.291 1.00 28.82 |
| ATOM | 764 CB VAL A 95 | 43.938 -11.737 106.677 1.00 30.75 |
| ATOM | 765 CG1 VAL A 95 | 43.745 -12.766 107.776 1.00 33.60 |
| MOTA | 766 CG2 VAL A 95 767 C VAL A 95 | 42.679 -11.611 105.849 1.00 24.87 |
| ATOM ATOM | | 45.503 -10.549 108.204 1.00 29.98 |
| ATOM | | 46.637 -10.649 107.729 1.00 31.36 |
| ATOM | 769 N SER A 96 770 CA SER A 96 | 45.264 -10.572 109.510 1.00 29.38 |
| ATOM | 771 CB SER A 96 | 46.335 -10.766 110.485 1.00 32.56 |
| ATOM | 772 OG SER A 96 | 47.325 -9.600 110.454 1.00 34.15 |
| ATOM | 773 C SER A 96 | 46 758 -8.448 111.051 1.00 28.33 |
| ATOM | 774 O SER A 96 | 45.681 ~10.804 111.854 1.00 32.10 |
| ATOM | 775 N TYR A 97 | 44 458 -10.839 111.950 1.00 37.91 46.484 -10.795 112.913 1.00 32.57 |
| ATOM | 776 CA TYR A 97 | |
| ATOM | 777 CB TYR A 97 | 46 605 33 77F 37F 300 4 55 55 5 |
| ATOM | 778 CG TYR A 97 | |
| ATOM | 779 CD1 TYR A 97 | |
| ATOM | 780 CE1 TYR A 97 | 47 000 48 |
| ATOM | 781 CD2 TYR A 97 | |
| ATOM | 782 CE2 TYR A 97 | |
| ATOM | 783 CE TYR A 97 | 46 010 |
| ATOM | 784 CH TYR A 97 | 16 777 4 |
| ATOM | 785 C TYR A 97 | 45 053 |
| ATCM | 786 0 TYR A 97 | 45 501 |
| ATOM | 787 N ALA A 98 | 46 115 |
| ATOM | 788 CA ALA A 98 | 46 048 |
| ATOM | 789 CE ALA A 98 | 47 105 |
| ATOM | 790 C ALA A .98 | 44.658 -6.533 113.962 1.00 30.35 |
| ATOM | 791 O ALA A 98 | 44.099 -5.655 114.612 1.00 31.82 |
| ATOM | 792 N MET A 99 | 44.094 -7.130 112.915 1.00 30.40 |
| - | | T. T. T. T. 00 30.40 |

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ATOM
           793
                CA
                    MET A
                           .99
                                     42.788
                                              -6.730 112.420
                                                               1.00 27.54
                                     42.370
 ATOM
           794
                CB
                    MET A
                            99
                                              -7.620 111.238
                                                               1.00 30.55
           795
 ATOM
                CG
                    MET A
                            99
                                     42.052
                                              -9.071 111.565
                                                               1.00 31.59
          796
 ATOM
                SD
                    MET A
                            99
                                     41.902
                                             -10.077 110.053
                                                               1.00 30.13
          797
 ATOM
                CE
                    MET A
                            99
                                     40.770
                                              -9.086 109.085
                                                               1.00 28.02
          798
 ATOM -
                C
                    MET A
                            99
                                     41.703
                                              -6.696 113.490
                                                               1.00 28.02
 ATOM
          799
                                     40.818
                0
                    MET A
                            99
                                              -5.842 113.446
                                                               1.00 24.53
                    PHE A 100
 ATOM
          800
                N
                                     41.752
                                             -7.614 114.449
                                                               1.00 26.07
 MOTA
          801
                CA
                                     40.759
                    PHE A 100
                                             -7.583 115.516
                                                               1.00 30.47
 ATOM
          802
                CB
                    -PHE A 100
                                     39.738
                                             -8.718 115.404
                                                               1.00 30.29
 MOTA
          803
                CG
                    PHE A 100
                                     38.693
                                             -8.657 116.475
                                                               1.00 29.35
 ATOM
          804
                CD1
                    PHE A. 100
                                     37.722
                                             -7.662 116.455
                                                               1.00 27.01
 MOTA
          805
                    PHE A 100
                CD2
                                     38.756
                                             -9.506 117.575-
                                                               1.00 30.68
 ATOM
          806
                CE1
                    PHE A 100
                                             -7.507 117.519
                                     36.834
                                                               1.00 31.41
 ATOM
          807
                CE2
                    PHE A 100
                                     37.873
                                             -9.356 118.644
                                                               1.00 28.39
          808
 MOTA
               CZ
                    PHE A 100
                                     36.913
                                             -8.355
                                                     118.618
                                                               1.00 24.06
 MOTA
          809
               C
                    PHE A 100
                                     41.345
                                             -7.616 116.922
                                                               1.00 29.67
 MOTA
          810
               0
                    PHE A 100
                                     41.028
                                             -6.751 117.740
                                                               1.00 29.67
 ATOM
          811
               N
                    THR A 101
                                     42.181
                                             -8.610 117.222
                                                               1.00 31.30
 MOTA
          812
               CA
                    THR A 101
                                     42.770
                                             -8.701 118.562
                                                               1.00 31.37
 MOTA
          813
               CB
                    THR A 101
                                             -9.977 118.732
                                     43.610
                                                               1.00 31.63
 ATOM
                    THR A 101
          814
               0G1
                                     42.777 -11.119
                                                               1.00 31.64
                                                     118.532
 MOTA
          815
               CG<sub>2</sub>
                    THR A 101
                                    44.197 -10.045
                                                    120.137
                                                               1.00 27.38
 MOTA
          816
               C
                    THR A 101
                                    43.647
                                             -7.493 118.884
                                                               1.00 31.66
 ATOM
          817
               0
                    THR A 101
                                    43.502
                                             -6.875
                                                    119.942
                                                              1.00 30.71
                    GLY A 102
 ATOM
         818
               N
                                             -7.166 117.976
                                    44.562
                                                              1.00 27.40
 ATOM
         819
               CA
                   GLY A 102
                                             -6.018 118.193
                                    45.430
                                                              1.00 27.19
 ATOM
         820
               С
                    GLY A 102
                                    44.631
                                             -4.728 118.266
                                                              1.00 27.26
                    GLY A 102
 ATOM
         821
               0
                                    44.785
                                             -3.940 119.201
                                                              1.00 27.68
         822
 MOTA
               N
                   SER A 103
                                    43.767
                                             -4.515 117.279
                                                              1.00 30.52
 ATOM
         823
               CA
                   SER A 103
                                             -3.314 117.216
                                    42.941
                                                              1.00
                                                                    31.91
 ATOM
         824
               CB
                   SER A 103
                                    42.085
                                             -3.334 115.949
                                                              1.00 34.63
 ATOM
         825
               OG
                   SER A 103
                                            -3.265 114.791
                                    42.896
                                                              1.00 35.94
 ATOM
         826
               С
                   SER A 103
                                            -3.163 118.441
                                    42.046
                                                              1.00
 ATOM
         827
               0
                   SER A 103
                                    41.891
                                            -2.065 118.984
                                                              1.00
ATOM
         828
              N
                   SER A 104
                                    41.455
                                             -4.270
                                                    118.871
                                                              1.00
                                                                   30.47
         829
ATOM
              CA
                   SER A 104
                                    40.584
                                            -4.251 120.038
                                                              1.00
                                                                   30.22
ATOM
         830
              CB
                   SER A 104
                                    39.978
                                            -5.633 120.265
                                                              1.00 23.88
ATOM
         831
              OG
                   SER A 104
                                    39.078
                                            -5.595
                                                    121.358
                                                              1.00
                                                                   36.91
ATOM
         832
              С
                   SER A 104
                                    41.367
                                            -3.841 121.282 - 1.00
                                                                   28.13
              O
ATOM
         833
                   SER A 104
                                    40.872
                                            -3.098
                                                    122.130
                                                              1.00 25.16
ATOM
         834
              N
                   LEU A 105
                                    42.594
                                            -4.336
                                                    121.386
                                                                   29.39
                                                              1.00
         835
                   LEU A 105
ATOM
              CA
                                    43.445
                                            -4.034 122.530
                                                              1.00 29.52
         836
              CB
                   LEU A 105
MOTA
                                    44.684
                                            -4.922 122.471
                                                              1.00 32.90
ATOM
         837
              CG
                   LEU
                      A 105
                                   45.461
                                            -5.176 123.754
                                                              1.00
                                                                   40.34
ATOM
         838
              CD1
                  LEU A 105
                                   44.520
                                            -5.723 124.828
                                                              1.00 35.95
         839
              CD2
MOTA
                  LEU A 105
                                   46.582
                                            -6.178 123.462
                                                              1.00 40.23
MOTA
        840
              С
                   LEU A 105
                                   43.834
                                            -2.552
                                                   122.511
                                                              1.00
                                                                   32.09
ATOM
        841
              0
                  LEU A 105
                                   43.896
                                            -1.894 123.554
                                                              1.00 30.38
                  ALA A 106
        842
MOTA
              N
                                   44.081
                                            -2.029 121.314
                                                              1.00 30.26
MOTA
        843
              CA
                  ALA A 106
                                   44.448
                                            -0.626 121.151
                                                              1.00
                                                                   28.31
                  ALA A 106
ATOM
        844
              CB
                                   44.958
                                            -0.386 119.738
                                                              1.00 23.88
        845
                  ALA A 106
MOTA
              C
                                   43.243
                                             0.268 121.434
                                                              1.00 26.04
ATOM
        846
              0
                  ALA A 106
                                   43.380
                                             1.376 121.952
                                                              1.00 20.63
              N
                  THR A 107
ATOM
        847
                                   42.058
                                            -0.224 121.099
                                                              1.00 26.86
                  THR A 107
        948
              CA
ATOM
                                   40.841
                                             0.542 121.322
                                                              1.00 25.04
ATOM
        849
              CB
                  THR A 107
                                   39,706
                                             0.007 120.443
                                                              1.00 26.50
                  THR A 107
        850
              OG1
МОТА
                                   40.111
                                             0.092 119.069
                                                              1.00 24.62
                  THR A 107
              CG2
MOTA
        851
                                   38.439
                                             0.824 120.629
                                                              1.00 19.80
        852
              С
                  THR A 107
                                             0.503 122.798
ATOM
                                   40.450
                                                              1.00 27.90
                  THR A 107
        853
             О
MOTA
                                   40.039
                                             1.515 123.361
                                                              1.00 29.04
                  GLY A 108
MOTA
        854
             N
                                   40.585
                                            -0.662 123.422
                                                             1.00 24.01
        855
             CA
                  GLY A 108
ATOM
                                   40.256
                                            -0.767 124.832
                                                             1.00 24.86
        856
             C
                  GLY A 108
MOTA
                                   41.181
                                            0.155 125.603
                                                             1.00 23.86
                  GLY A 108
        857
             0
                                            0.790 126.572
                                                             1.00 26.97
ATOM
                                   40.771
        858
                  SER A 109
ATCM
                                   42.434
                                             0.236 125.158
                                                             1.00 23.07
```

| ATOM | 859 CA SER A 109 | 43.421 | 1.090 125.807 | 1 00 20 00 |
|--------------|--------------------|----------|----------------|------------|
| ATOM | 860 CB SER A 109 | 44.795 | | |
| ATOM | 861 OG SER A 109 | | 0.910 125.160 | |
| | | 45.294 | -0.393 125.402 | |
| ATOM | | 43.008 | 2.552 125.759 | 1.00 21.13 |
| ATOM | 863 O SER A 109 | 43.323 | 3.312 126.672 | 1.00 23.17 |
| MOTA | 864 N THR A 110 | 42.311 | 2.949 124.698 | 1.00 20.83 |
| MOTA | 865 CA THR A 110 | 41.841 | 4.327 124.583 | 1.00 21.84 |
| ATOM | 866 CB THR A 110 | 41.332 | 4.648 123.161 | |
| ATOM | 867 OG1 THR A 110 | | | 1.00 24.33 |
| | | 42.452 | 4.769 122.276 | 1.00 25.38 |
| MOTA | 868 CG2 THR A 110 | 40.543 | 5.954 123.144 | 1.00 21.18 |
| MOTA | 869 C THR A 110 | 40.725 | 4.561 125.600 | 1.00 28.52 |
| MOTA | 870 O THR A 110 | 40.632 | 5.637 126.197 | 1.00 28.27 |
| MOTA | 871. N VAL A 111 | 39.882 | 3.558 125.809 | 1.00 26.88 |
| ATOM . | 872 CA VAL A 111 | 38.811 | 3.706 126.793 | |
| ATOM | 873 CB VAL A 111 | 37.820 | 2.519 126.742 | 1.00 30.04 |
| MOTA | 874 CG1 VAL A 111 | | 2.519 126.742 | 1.00 29.94 |
| ATOM | 875 CG2 VAL A 111 | 36.737 | 2.693 127.802 | 1.00 27.07 |
| | | 37.193 | 2.431 125.355 | 1.00 25.26 |
| ATOM | 876 C VAL A 111 | 39.440 | 3.797 128.187 | 1.00 28.10 |
| MOTA | 877 O VAL A 111 | 38.968 | 4.539 129.039 | 1.00 26.06 |
| MOTA | 878 N GLNA 112 | 40.521 | 3.056 128.415 | 1.00 23.92 |
| ATOM | 879 CA GLN A 112 | 41.188 | 3.097 129.711 | 1.00 30.27 |
| MOTA | 880 CB GLN A 112 | 42.268 | 2.020 129.804 | |
| ATOM | 881 CG GLN A 112 | 41.777 | 0.629 129.481 | 1.00 28.61 |
| ATOM | 882 CD GLN A 112 | 42.883 | 0.029 129.461 | 1.00 28.90 |
| MOTA | 883 OE1 GLN A 112 | | -0.397 129.564 | 1.00 28.60 |
| | | 43.344 | -0.740 130.653 | 1.00 29.68 |
| MOTA | 884 NE2 GLN A 112 | 43.333 | -0.880 128.409 | 1.00 22.13 |
| ATOM | 885 C GLN A 112 | 41.834 | 4.461 129.931 | 1.00 29.99 |
| ATOM | 886 O GLN A 112 | 41.791 | 5.006 131.035 | 1.00 28.43 |
| ATOM | 887 N ALA A 113 | 42.453 | 5.004 128.885 | 1.00 28.64 |
| MOTA | 888 CA ALA A 113 | 43.083 | 6.315 129.001 | 1.00 26.62 |
| ATOM | 889 CB ALA A 113 | 43.693 | 6.732 127.684 | 1.00 23.49 |
| ATOM | 890 C ALA A 113 | 42.005 | | _ |
| ATOM | 891 O ALA A 113 | 42.232 | | 1.00 24.63 |
| ATOM | 892 N ILE A 114 | | 8.183 130.240 | 1.00 26.38 |
| | | 40.824 | 7.163 128.822 | 1.00 25.26 |
| ATOM | | 39.728 | 8.063 129.145 | 1.00 27.05 |
| ATOM | 894 CB ILE A 114 | 38.554 | 7.887 128.156 | 1.00 26.93 |
| ATOM | 895 CG2 ILE A 114 | 37.387 | 8.770 128.576 | 1.00 25.86 |
| ATOM | 896 CG1 ILE A 114 | 39.008 | 8.259 126.739 | 1.00 28.38 |
| ATOM | 897 CD1 ILE A 114 | 37.938 | 8.105 125.669 | 1.00 28.64 |
| ATOM | . 898 C ILE A 114 | 39.239 | 7.823 130.578 | 1.00 31.36 |
| ATOM | 899 O ILE A 114 | 38.898 | 8.770 131.291 | 1.00 24.56 |
| ATOM | 900 N GLU A 115 | 39.210 | 6.563 131.005 | |
| ATOM | 901 CA GLU A 115 | | | 1.00 31.17 |
| ATOM | | 38.750 | 6.257 132.358 | 1.00 32.12 |
| | | 38.729 | 4.744 132.607 | 1.00 32.15 |
| ATOM | 903 CG GLU A 115 | 37.904 | 3.947 131.598 | 1.00 32.84 |
| ATOM | 904 CD GLU A 115 | 37.875 | 2.459 131.912 | 1.00 34.12 |
| ATOM | 905 OE1 GLU A 115 | 38.910 | 1.910 132.345 | 1.00 30.36 |
| ATOM | 906 OE2 GLU A 115 | 36.826 | 1.827 131.699 | 1.00 31.38 |
| ATOM | 907 C GLU A 115 | 39.675 | 6.932 133.357 | 1.00 31.65 |
| ATOM | 908 O GLU A 115 | 39.224 | 7.446 134.383 | 1.00 29.25 |
| ATOM | 909 N GLU A 116 | 40.970 | 6.933 133.053 | |
| ATOM | 910 CA GLU A 116 | 41.942 | | 1.00 31.50 |
| | | | 7.564 133.934 | 1.00 32.34 |
| ATOM | | 43.367 | 7.285 133.457 | 1.00 33.29 |
| ATOM | ·912 CG GLU A 116 | 43.805 | 5.842 133.633 | 1.00 32.29 |
| atom | 913 CD GLU A 116 | 43.701 | 5.378 135.079 | 1.00 36.87 |
| ATOM | 914 OE1 GLU A 116. | 44.329 | 6.003 135.961 | 1.00 34.07 |
| ATOM | 915 OE2 GLU A 116 | 42.993 | 4.385 135.335 | 1.00 35.00 |
| ATOM | 916 C GLU A 116 | 41.702 | 9.067 134.006 | 1.00 36.69 |
| ATOM | 917 O GLU A 116 | 41.863 | 9.678 135.066 | 1.00 34.39 |
| ATOM | 918 N PHE A 117 | 41.317 | 9.661 132.881 | |
| ATOM ATOM | 919 CA PHE A 117 | | | 1.00 31.19 |
| | | . | | 1.00 28.43 |
| MOTA | 920 CB PHE A 117 | | 11.509 131.444 | 1.00.30.14 |
| ATOM | 921 CG PHE A 117 | | 12.908 131.381 | 1.00 35.78 |
| ATOM | 922 CD1 PHE A 117 | | 4.006 131.501 | 1.00 33.39 |
| ROM | 923 CD2 PHE A 117 | 38.675] | 3.123 131.225 | 1.00 38.90 |
| MOTA | 924 CE1 PHE A 117 | | 5.299 131.466 | 1.00 30.65 |
| | | _ | | |

| _ | | | | | | | | | | |
|--------------|-------------|------------|------------------|----------------|----------------|------|----------------|--------------------|----------------|----------------|
| ATOM | 925 | | E2 PHE . | A 117 | 38. | 153 | | 2 131.190 | | 36.50 |
| MOTA | 926 | | | A 117 | 39. | 003 | | 1 131.310 | | 35.41 |
| ATOM | 927 | | | A 117 | | 908 | 11.40 | | | 32.78 |
| MOTA | 928 | | | A 117 | | 966 | | 7 134.566 | | 29.82 |
| ATOM | 929 | | | A 118 | | 874 | | 3 133.771 | | 28.61 |
| ATOM | 930 931 | | 1 LEU / | A 118 A 118 | 37. | | | 134.632 | | 32.00 |
| ATOM ATOM | 932 | | DEU A | A 118 | 36. | | 9.748 | 3 134.263 | | 29.19 |
| ATOM | 933 | | Ol LEU A | 1.110 | 36. 34. | | 9.830 | 132.820 132.622 | | 34.47 |
| ATOM | 934 | | | | 35. | | | 132.522 | | 32.69 32.24 |
| ATOM | . 935 | | LEU A | | 38. | | | 136.094 | | 31.17 |
| ATOM | 936 | | LEU A | | 37 : . | | | 136.964 | 1 00 | 28.32 |
| MOTA | 937 | N | LYS A | | 39. | | | 136.363 | | 27.23 |
| ATOM | 938 | CA | LYS A | 119 | 39. | | | 137.733 | | 30.95 |
| MOTA | 939 | | | | 40.2 | 203 | | 137.884 | 1.00 | 26.35 |
| ATOM | 940 | | | | 39.2 | | | 137.540 | 1.00 | 32.44 |
| MOTA | 941 | CD | | | 39.8 | | | 137.986 | | 33.31 |
| MOTA | 942 | | | | 41.2 | | | 137.411 | | 33.47 |
| MOTA | 943 944 | NZ C | | | 41.8 | | | 137.904 | | 33.40 |
| MOTA MOTA | 945 | 0 | LYS A | | 40.4 41.0 | | 10.594 | 138.173 139.270 | | 32.65 |
| ATOM | 946 | N | GLY A | | 40.6 | | | 139.270 | | 28.83 |
| ATOM | 947 | CA | | | 41.5 | | | 137.652 | | 33.77 33.84 |
| ATOM | 948 | С | GLY A | | | | 12.448 | | | 34.27 |
| ATOM | 949 | 0 | GLY A | | 43.8 | | | 137.776 | | 36.80 |
| ATOM | 950 | N | ASN A | | 43.3 | | | 136.606 | | 30.77 |
| MOTA | 951 | CA | ASN A | | 44.7 | | | 136.244 | 1.00 | 31.73 |
| MOTA | 952 | CB | ASN A | | 45.0 | | | 136.437 | | 29.34 |
| ATOM | 953 | CG | ASN A | | 44.8 | | | 137.851 | 1.00 | 35.83 |
| MOTA | 954 | OD1 | | | . 45.1 | | 9.861 | | | 32.74 |
| ATOM ATOM | 955 956 | ND2 | A NSA S A NSA | | 44.3 44.9 | | | 137,986 | | 33.20 |
| MOTA | 957 | ō | ASN A | | 44.0 | | 11.952 | 134.790 134.110 | | 32.59 |
| ATOM | 958 | N | VAL A | | 46.1 | | | 134.110 | 1.00 | 34.69 32.74 |
| MOTA | 959 | CA | VAL A | | 46.5 | | | 132.946 | | 33.59 |
| MOTA | 960 | CB | VAL A | | 47.5 | | | 132.882 | | 36.05 |
| MOTA | 961 | CG1 | | | 47.8 | 84 1 | 13.121 | 131.438 | | 37.58 |
| MOTA | 962 | CG2 | | | 47.0 | | 14.021 | | | 37.19 |
| ATOM | 963 | C | VAL A | | 47.1 | | 10.397 | | | 34.47 |
| MOTA | 964 965 | Ŋ | VAL A | | 48.0 | | 9.801 | | | 31.28 |
| ATOM ATOM | 966 | CA | ALA A ALA A | | 46.6 47.1 | | 9.989 8.784 | | | 28.06 |
| ATOM | 967 | CB | ALA A | | 46.1 | | 7.666 | | | 30.73 32.69 |
| ATOM | 968 | C | ALA A | | 47.4 | | 8.969 | | | 30.55 |
| MOTA | 969 | 0 | ALA A | | 46.9 | | 9.830 | | | 32.89 |
| ATOM | 970 | N | PHE A | | 48.3 | 80 | 8.136 | 128.613 | 1.00 | |
| MOTA | 971 | CA | PHE A | | 48.8 | | 8.157 | 127.229 | 1.00 | 26.56 |
| ATOM | 972 | CB | PHE A | | 50.2 | | | 127.157 | 1.00 | |
| ATOM | 973 | CG | PHE A | | 50.9 | | | 125.793 | 1.00 | |
| MOTA | 974 975 | CD1 | PHE A | | 50.1 | | 8.785 | 124.629 | 1.00 | |
| MOTA MOTA | 976 | | PHE A | | 52.20 50.80 | | | 125.686 123.385 | $1.00 \\ 1.00$ | |
| ATOM | 977 | | | | 52.8 | | | 124.449 | 1.00 | |
| ATOM | 978 | CZ | PHE A | | 52.10 | - | | 123.296 | 1.00 | |
| ATOM | 979 | С | PHE A | | 48.6 | | 6.749 | 126.675 | 1.00 | |
| MOTA | 9 80 | 0 | PHE A | 124 | 49.18 | 31 | | 127.260 | 1.00 | |
| ATOM | 981 | N | ASN A | | 47.93 | 33 | 6.624 | 125.580 | 1.00 | |
| MOTA | 982 | CA | ASN A | | 47.75 | | | 124.905 | 1.00 | |
| MOTA | 983 | CB | ASN A | | 46.27 | | | 124.756 | 1.00 | |
| ATOM | 984 | CG | ASN A | | 46.07 | _ | 3.784 | 123.856 | 1.00 | |
| ATOM | 985 986 | OD1 ND2 | ASN A ASN A | | 46.91 44.96 | | | 123.822 | 1.00 | |
| ATOM | 987 | C | ASN A | | 44.38 | | | 123.138 123.518 | 1.00 | |
| ATOM ATOM | 988 | õ | ASN A | | 47.71 | | | 122.542 | 1.00 2 | |
| ATOM | 989 | N | PRO A | | 49.68 | | | 123.423 | 1.00 2 | |
| ATOM | 990 | CD | PRO A | | 50.58 | | | 124.519 | 1.00 | |
| | | | | | | | | | | |

|)TA | OM 991 CA PRO A 126 | 50.413 | ·5.130 122.160 | 1.00 22.39 |
|-------|----------------------|---------|--------------------------------|--------------|
| ATC | OM 992 CB PRO A 126 | 51.829 | | |
| ATC | | 51.023 | | |
| | | 51.564 | | 3 1.00 25.43 |
| ATC | | 49.867 | 4.224 121.058 | 3 1.00 23.18 |
| ATC | OM 995 O PRO A 126 | 50.173 | | |
| ATO | | | | |
| | | 49.058 | 3.232 121.423 | 1.00 23.27 |
| ATC | M 997 CA ALA A 127 | 48.493 | 2.306 120.444 | |
| OTA | | 48.176 | | |
| | | | 0.967 121.118 | |
| ATC | | 47.241 | 2.864 119.778 | 1.00 24.76 |
| ATC | M 1000 O ALA A 127 | 46.806 | 2.360 118.745 | |
| ATC | | 46.666 | | |
| | | | 3.906 120.367 | |
| ATC | | 45.461 | 4.494 119.809 | 1.00 21.43 |
| · ATC | M 1003 C GLY A 128 | 45.732 | 5.521 118.725 | 1.00 23.55 |
| ATC | | 46.875 | 5.001 110.723 5.005 110.001 | |
| ** | | 40.075 | 5.695 118.291 | |
| ATC | | 44.680 | 6.199 118.283 | 1.00 18.03 |
| ATO | M 1006 CA GLY A 129 | 44.822 | 7.205 117.243 | 1.00 24.99 |
| ATO | M 1007 C GLY A 129 | 44.600 | 6 655 117 243 | |
| | | 44.600 | 6.655 115.847 | |
| ATO | | 44.963 | 7.293 114.857 | 1.00 24.99 |
| OTA | M 1009 N MET A 130 | 44.002 | 5.470 115.765 | 1.00 20.01 |
| ATO | | 43.729 | 4 005 114 401 | |
| | | | 4.825 114.481 | |
| ATO | | 43.360 | 3.361 114.744 | 1.00 22.77 |
| ATO: | M 1012 CG MET A 130 | 44.455 | 2.661 115.563 | 1.00 26.30 |
| ATO | | 44.198 | 0.913 115.989 | |
| ATO | | | 0.913 115.989 | |
| | | 42.665 | 1.030 116.936 | 1.00 27.59 |
| ATO | M 1015 C MET A 130 | 42.580 | 5.617 113.869 | 1.00 23.70 |
| ATO | | 41.421 | 5.199 113.901 | |
| ATO | | | 3.199 113.901 | 1.00 26.28 |
| | | 42.926 | 6.766 113.294 | 1.00 20.66 |
| ATO | 1 1018 CA HIS A 131 | 41.933 | 7.687 112.775 | 1.00 20.99 |
| ATO | 1 1019 CB HIS A 131 | 42.474 | 9.125 112.891 | 1.00 21.01 |
| ATO | | 43.699 | | |
| | _ | | 9.391 112.069 | 1.00 28.30 |
| ATO | | 44.498 | 8.549 111.373 | 1.00 19.65 |
| ATON | 1 1022 ND1 HIS A 131 | 44.246 | 10.649 111.917 | 1.00 27.76 |
| MOTA | 1 1023 CE1 HIS A 131 | 45.328 | 10.567 111.163 | |
| ATON | | | | 1.00 20.48 |
| | | 45.503 | 9.302 110.820 | 1.00 24.18 |
| ATOM | | 41.280 | 7.513 111.416 | 1.00 23.76 |
| ATOM | 1026 O HIS A 131 | 40.453 | 8.341 111.051 | 1.00 21.95 |
| ATOM | | | | |
| | | 41.600 | 6.449 110.682 | 1.00 25.12 |
| ATOM | | 41.006 | 6.257 109.354 | 1.00 23.32 |
| ATOM | 1029 CB HIS A 132 | 42.060 | 5.715 108.388 | 1.00 17.87 |
| ATOM | 1030 CG HIS A 132 | 43.148 | 6.689 108.072 | 1.00 17.07 |
| ATOM | | | 0.689 108.072 | 1.00 24.79 |
| | | 44.496 | 6.574 108.144 | 1.00 21.72 |
| MOTA | | 42.896 | 7.944 107.556 | 1.00 13.58 |
| ATOM | 1033 CE1 HIS A 132 | 44.044 | 8.558 107.323 | 1.00 15.41 |
| ATOM | | | | |
| | | 45.028 | 7.748 107.668 | 1.00 15.27 |
| ATOM | | 39.752 | 5.386 109.208 | 1.00 23.38 |
| ATOM | 1036 O HIS A 132 | 38.947 | 5.615 108.304 | 1 00 24.70 |
| ATOM | 1037 N ALA A 133 | 39.587 | 4.388 110.070 | - 00 24.70 |
| | | | 4.388 110.070 | 1.00 23.34 |
| ATOM | 1038 CA ALA A 133 | 38.453 | 3.471 109.953 | 2 00 23.77 |
| MOTA | 1039 CB ALA A 133 | 38.515 | 2.417 111.053 | 1.00 27.49 |
| ATOM | 1040 C ALA A 133 | 37.093 | 4.145 109.966 | _ |
| ATOM | | | = 117 107 700 | 1.00 23.02 |
| | | 36.878 | 5.117 110.691 | 1.00 25.98 |
| ATOM | 1042 N PHE A 134 | 36.179 | 3.633 109.148 | 1.00 18.90 |
| ATOM | 1043 CA PHE A 134 | 34.831 | 4.173 109.103 | |
| ATOM | 1044 CB PHE A 134 | | | 1.00 23.73 |
| | | 34.317 | 4.296.107.663 | 1.00 24.29 |
| ATOM | 1045 CG PHE A 134 | 35.119 | 5.225 106.801 | 1.00 26.67 |
| ATOM | 1046 CD1 PHE A 134 | 36.025 | 4.724 105.867 | 1.00 28.69 |
| ATOM | 1047 CD2 PHE A 134 | 34.975 | | |
| | | | 6.605 106.921 | 1.00 32.49 |
| MOTA | 1048 CE1 PHE A 134 | 36.775 | 5.582 105.063 | 1.00 28.65 |
| ATOM | 1049 CE2 PHE A 134 | 35.724 | 7.479 106.119 | 1.00 27.86 |
| ATOM | 1050 CZ PHE A 134 | 36.623 | | |
| | | | 6.967 105.188 | 1.00 23.93 |
| MOTA | 1051 C PHE A 134 | 33.894 | 3.260 109.884 | 1.00 25.91 |
| ATOM | 1052 O PHE A 134 | 34.270 | 2.172 110.319 | 1.00 27.20 |
| ATOM | 1053 N LYS A 135 | 32.670 | | |
| | | | 3.728 110.062 | 1.00 29.14 |
| ATOM | | 31.638 | 2.984 110.765 | 1.00 35.26 |
| ATOM | 1055 CB LYS A 135 | 30.294 | 3.628 110.429 | 1.00 35.86 |
| ATOM | 1056 CG LYS A 135 | 29.072 | 2.779 110.667 | 1.00 46.26 |
| | · · · | | 2.775 110.007 | 1.00 40.20 |
| | | | | |

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Figure 18-17

| ATOM | 1057 | 7 CD LYS A 135 | 27.834 | 3.542 110.211 | 1.00 47.72 |
|--------|--------|---------------------------------------|----------------|----------------|------------|
| ATOM | 1058 | 3 CE LYS A 135 | 26.610 | 2.645 110.169 | 1.00 53.65 |
| ATOM | 1059 | | 26.788 | | 1.00 53.27 |
| | | | | | |
| ATOM | 1060 | | 31.617 | | 1.00 35.62 |
| ATOM | 1061 | O LYS A 135 | 31.609 | 0.635 111.301 | 1.00 32.58 |
| ATOM- | 1062 | N SER A 136 | 31.629 | 1.180 109.122 | 1.00 35.97 |
| ATOM | 1063 | CA SER A 136 | 31.555 | -0.211 108.684 | 1.00 38.99 |
| ATOM | 1064 | | | -0.474 108.083 | |
| | | | 30.172 | | 1.00 38.87 |
| MOTA | 1065 | | 29.146 | -0.072 108.975 | 1.00 43.54 |
| ATOM | 1066 | C -SER A 136 | 32.608 | -0.616 107.660 | 1.00 37.84 |
| ATOM | 1067 | O SER A 136 | 32.350 | -1.491 106.828 | 1.00 36.33 |
| ATOM | 1068 | | 33.788 | -0.008 107.705 | 1.00 33.23 |
| | | | | | |
| MOTA | 1069 | | 34.797 | -0.368 106.724 | 1.00 30.89 |
| MOTA | 1070 | | 34.456 | 0.291 105.385 | 1.00 33.88 |
| MOTA | - 1071 | CG ARG A 137 | 35.009 | -0.465 104.201 | 1.00 44.41 |
| MOTA | 1072 | CD ARG A 137 | 34.809 | 0.261 102.880 | 1.00 46.27 |
| MOTA | 1073 | | 35.091 | -0.645 101.768 | 1.00 48.87 |
| | 1074 | | | | |
| MOTA | | | 35.352 | -0.261 100.526 | 1.00 48.64 |
| MOTA | 1075 | | 35.372 | 1.029 100.220 | 1.00 51.82 |
| ATOM | 1076 | NH2 ARG A 137 | 35.592 | -1.169 99.589 | 1.00 49.01 |
| ATOM | 1077 | C ARG A 137 | 36.209 | 0.021 107.143 | 1.00 31.84 |
| ATOM | 1078 | O ARG A 137 | 36.428 | 1.079 107.742 | 1.00 30.36 |
| | 1079 | | | | |
| MOTA | | N ALA A 138 | 37.166 | -0.845 106.828 | 1.00 30.06 |
| ATOM | 1080 | CA ALA A 138 | 38.560 | -0.588 107.158 | 1.00 32.24 |
| ATOM | 1081 | CB ALA A 138 | 39.367 | -1.864 107.048 | 1.00 31.25 |
| ATOM | 1082 | C ALA A 138 | 39.095 | 0.449 106.187 | 1.00 29.49 |
| MOTA | 1083 | O ALA A 138 | 38.612 | 0.551 105.063 | 1.00 26.11 |
| | 1084 | N ASN A 139 | | | |
| MOTA | | | 40.099 | 1.206 106.615 | 1.00 29.54 |
| ATOM | 1085 | CA ASN A 139 | 40.673 | 2.241 105.767 | 1.00 26.99 |
| ATOM | 1086 | CB ASN A 139 | 39.685 | 3.415 105.662 | 1.00 24.10 |
| ATOM | 1087 | CG ASN A 139 | 40.209 | 4.556 104.811 | 1.00 28.02 |
| ATOM | 1088 | OD1 ASN A 139 | 40.729 | 4.334 103.727 | 1.00 26.90 |
| ATOM | 1089 | ND2 ASN A 139 | 40.050 | 5.789 105.293 | 1.00 23.55 |
| | | | | | |
| ATOM | 1090 | C ASN A 139 | 42.027 | 2.713 106.285 | 1.00 30.17 |
| ATOM | 1091 | 0 ASN A 139 | 42.245 | 2.827 107.497 | 1.00 27.55 |
| ATOM | 1092 | N GLY A 140 | 42.944 | 2.959 105.354 | 1.00 31.82 |
| ATOM | 1093 | CA GLY A 140 | 44.277 | 3.428 105.702 | 1.00 24.90 |
| ATOM | 1094 | C GLY A 140 | 45.000 | 2.696 106.816 | 1.00 27.79 |
| ATOM | 1095 | O GLY A 140 | 45.560 | 3.339 107.705 | 1.00 23.85 |
| | 1096 | | | | |
| ATOM | | | 45.006 | 1.365 106.768 | 1.00 24.35 |
| MOTA | 1097 | CA PHE A 141 | 45.679 | 0.538 107.783 | 1.00 24.53 |
| ATOM | 1098 | CB PHE A 141 | 47.031 | 1.146 108.197 | 1.00 26.40 |
| ATOM | 1099 | CG PHE A 141 | 47.997 | 1.366 107.062 | 1.00 30.31 |
| ATOM | 1100 | CD1 PHE A 141 | 49.145 | 2.125 107.269 | 1.00 31.60 |
| ATOM | 1101 | CD2 PHE A 141 | 47.781 | 0.811 105.802 | 1.00 29.44 |
| | | | | | |
| ATOM | 1102 | CE1 PHE A 141 | 50.06 6 | 2.331 106.243 | 1.00 30.44 |
| MOTA | 1103. | | 48.694 | 1.008 104.770 | 1.00 27.91 |
| ATOM | 1104 | CZ PHE A 141 | 49.840 | 1.771 104.991 | 1.00 29.38 |
| ATOM | 1105 | C PHE A 141 | 44.846 | 0.387 109.056 | 1.00 23.53 |
| MOTA | 1106 | O PHE A 141 | 45.194 | -0.399 109.941 | 1.00 23.09 |
| | 1107 | N CYS A 142 | 43.760 | 1.143 109.159 | 1.00 22.86 |
| MOTA | | 12 CIS W 147 | | | |
| MOTA | 1108 | CA CYS A 142 | 42.925 | 1.099 110.356 | 1.00 23.87 |
| MOTA | 1109 | CB CYS A 142 | 42.472 | 2.516 110.723 | 1.00 22.51 |
| ATOM | 1110 | SG CYS A 142 | 43.828 | 3.683 111.072 | 1.00 27.62 |
| ATOM | 1111 | C CYS A 142 | 41.694 | 0.205 110.233 | 1.00 24.20 |
| ATOM | 1112 | O CYS A 142 | 40.932 | 0.307 109.272 | 1.00 24.12 |
| | | | | | |
| MOTA | 1113 | N TYR A 143 | 41.498 | -0.663 111.219 | 1.00-23.84 |
| ATOM | 1114 | CA TYR A 143 | 40.335 | -1.546 111.236 | 1.00 26.07 |
| ATOM | 1115 | CB TYR A 143 | 40.728 | -2.958 111.680 | 1.00 27.89 |
| ATOM | 1116 | CG TYR A 143 | 41.829 | -3.582 110.855 | 1.00 27.30 |
| ATOM | 1117 | CD1 TYR A 143 | 43.169 | -3.329 111.137 | 1.00 25.76 |
| | 1118 | CE1 TYR A 143 | 44.185 | -3.875 110.346 | 1.00 25.77 |
| ATOM | | | | | |
| MOTA | 1119 | CD2 TYR A 143 | 41.526 | -4.394 109.762 | 1.00 25.87 |
| ATOM ' | 1120 | CE2 TYR A 143 | 42.531 | -4.941 108.967 | 1.00 23.10 |
| MOTA | 1121 | CZ TYR A 143 | 43.854 | -4.679 109.262 | 1.00 22.93 |
| ATOM | 1122 | OH TYR A 143 | 44.849 | -5.217 108.476 | 1.00 20.64 |
| ••• | _ | · · · · · · · · · · · · · · · · · · · | | | |

| MOTA | 1123 C TYR A 143 | 39.281 | -0.991 112.193 | 1.00 24.56 |
|--------------|---------------------------------------|------------------|--------------------------------|------------|
| MCTA | 1124 O TYR A 143 | 38.085 | | 1.00 24.88 |
| MOTA | 1125 N ILE A 144 | 39.734 | | 1.00 23.77 |
| ATOM | 1126 CA ILE A 144 | 38.833 | | 1.00 27.11 |
| ATOM | 1127 CB ILE A 144 | 38.871 | | 1.00 27.11 |
| ATOM | 1128 CG2 ILE A 144 | 37.941 | | |
| ATOM | 1129 CG1 ILE A 144 | 38.430 | 2 160 116 346 | |
| | 1130 CD1 ILE A 144 | | | |
| MOTA | | 38.535 | | 1.00 28.70 |
| ATOM | 1131 C ILE A 144 | 39.248 | | |
| ATOM | 1132 O ILE A 144 | 40.428 | 1.843 114.800 | |
| ATOM | 1133 N ASN A 145 | 38.277 | 2.453 114.669 | |
| ATOM | 1134 CA ASN A 145 | 38.555 | 3.866 114.920 | |
| MOTA | 1135 CB ASN A 145 | 37.559 | 4.732 114.133 | 1.00 18.87 |
| MOTA | 1136 CG ASN A 145 | 37.956 | 6.205 114.091 | 1.00 22.21 |
| ATOM | 1137 OD1 ASN A 145 | 38.223 | 6.823 115.124 | 1.00 22.47 |
| ATOM | 1138 ND2 ASN A 145 | 37.978 | 6.776 112.892 | 1.00 23.78 |
| ATOM | 1139 C ASN A 145 | 38.417 | 4.141 116.418 | 1.00 22.63 |
| MOTA | 1140 O ASN A 145 | 37.338 | 4.535 116.880 | 1.00 22.45 |
| ATOM | 1141 N ASN A 146 | 39.495 | 3.941 117.178 | 1.00 16.63 |
| MOTA | 1142 CA ASN A 146 | 39.423 | 4.160 118.628 | 1.00 23.57 |
| ATOM | 1143 CB ASN A 146 | 40.708 | 3.678 119.320 | 1.00 19.80 |
| MOTA | 1144 CG ASN A 146 | 41.924 | 4.508 118.967 | 1.00 27.81 |
| MOTA | 1145 OD1 ASN A 146 | 42.299 | 5.421 119.704 | 1.00 19.55 |
| ATOM | 1146 ND2 ASN A 146 | 42.544 | 4.202 117.827 | 1.00 19.55 |
| MOTA | 1147 C ASN A 146 | 39.079 | 5.602 119.023 | 1.00 26.32 |
| MOTA | 1148 O ASN A 146 | 38.452 | 5.827 120.059 | 1.00 28.34 |
| MOTA | 1149 N PRO A 147 | 39.512 | 6.605 118.231 | 1.00 28.46 |
| ATOM | 1150 CD PRO A 147 | 40.383 | 6.637 117.042 | 1.00 27.18 |
| ATOM | 1151 CA PRO A 147 | 39.150 | 7.972 118.618 | 1.00 24.15 |
| MOTA | 1152 CB PRO A 147 | 39.859 | 8.815 117.558 | 1.00 25.13 |
| MOTA | 1153 CG PRO A 147 1154 C PRO A 147 | 41.081 | 7.959 117.235 | 1.00 30.05 |
| ATOM | | 37.618 | 8.136 118.578 | 1.00 26.71 |
| MOTA | | 37.017 | 8.760 119.456 | 1.00 24.93 |
| MOTA | 1156 N ALA A 148 1157 CA ALA A 148 | 36.989 | 7:557 117.562 | 1.00 21.42 |
| ATOM | 1158 CB ALA A 148 | 35.536 35.112 | 7.633 117.416 7.044 116.072 | 1.00 21.03 |
| MOTA MOTA | 1156 CB ALA A 148 | 34.838 | | 1.00 19.98 |
| ATOM | 1160 O ALA A 148 | 33.822 | 6.891 118.552 7.344 119.067 | 1.00 20.49 |
| ATOM | 1161 N VAL A 149 | 35.381 | 5.739 118.928 | 1.00 21.44 |
| ATOM | 1162 CA VAL A 149 | 34.818 | 4.950 120.016 | 1.00 19.20 |
| ATOM | 1163 CE VAL A 149 | 35.570 | 3.608 120.181 | 1.00 25.96 |
| ATOM | 1164 CG1 VAL A 149 | 35.158 | 2.918 121.485 | 1.00 25.38 |
| ATOM | 1165 CG2 VAL A 149 | 35.262 | 2.704 118.995 | 1.00 25.67 |
| ATOM | 1166 C VAL A 149 | 34.947 | 5.752 121.304 | 1.00 23.56 |
| MOTA | 1167 O VAL A 149 | 33.990 | 5.887 122.064 | 1.00 23.50 |
| ATOM | 1168 N GLY A 150 | 36.143 | 6.287 121.536 | 1.00 24.65 |
| ATOM | 1169 CA GLY A 150 | 36.390 | 7.074 122.731 | 1.00 22.82 |
| ATOM | 1170 C GLY A 150 | 35.477 | 8.281 122.838 | 1.00 25.46 |
| ATOM | 1171 O GLY A 150 | 34.919 | 8.564 123.904 | 1.00 23.17 |
| ATOM | 1172 N ILE A 151 | 35.327 | 9.001 121.733 | 1.00 24.38 |
| ATOM | 1173 CA ILE A 151 | | 10.180 121.716 | |
| ATOM | 1174 CB ILE A 151 | 34.610 | 10.928 120.371 | 1.00 24.45 |
| ATOM | 1175 CG2 ILE A 151 | 33.598 | 12.077 120.306 | 1.00 24.71 |
| ATOM | 1176 CG1 ILE A 151 | 36.041 | 11.462 120.222 | 1.00 28.02 |
| ATOM | 1177 CD1 ILE A 151 | 36.354 | 12.056 118.854 | 1.00 27.10 |
| ATOM | 1178 C ILE A 151 | 33.018 | 9.806 121.987 | 1.00 28.19 |
| ATOM | 1179 O ILE A 151 | 32.337 | 10.482 122.763 | 1.00 26.37 |
| ATOM | 1180 N GLU A 152 | 32.532 | 8.734 121.364 | 1.00 26.32 |
| ATOM | 1181 CA GLU A 152 | 31.149 | 8.314 121.601 | 1.00 30.07 |
| ATOM | 1182 CB GLU A 152 | 30.758 | 7.161 120.672 | 1.00 29.37 |
| ATOM | 1183 CG GLU A 152 | 30.609 | 7.543 119.194 | 1.00 27.68 |
| ATOM | 1184 CD GLU A 152 | 29.455 | 8.504 118.946 | 1.00 31.82 |
| ATOM | 1185 OE1 GLU A 152 | 29.139 | 8.777 117.773 | 1.00 33.51 |
| ATOM · | 1186 OE2 GLU A 152 | 28.862 | 9.009 119.918 | 1.00 34.73 |
| ATOM | 1187 C GLU A 152 | 31.009 | 7.879 123.055 | 1.00 28.00 |
| ATOM | 1188 O GLU A 152 | 29.980 | 8.096 123.683 | 1.00 31.23 |
| | | | | |

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| | | • |
|--------------|---------------------------------------|--|
| ATO | M 1189 N TYR A 153 | 32.054 7.253 123.583 1.00 28 7 |
| ATO: | M 1190 CA TYR A 153 | 32 066 6 005 124 054 |
| ATO] | M 1191 CB TYR A 153 | 22 408 6 22 22 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| ATOI | M 1192 CG TYR A 153 | 23 617 5 030 405 307 1.00 31.30 |
| ATO | M 1193 CD1 TYR A 153 | 22 11 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| ATO | M 1194 CE1 TYR A 153 | 37 321 4 200 400 53.43 |
| ATO1 | | 34 330 |
| ATON | M 1196 CE2 TYR A 153 | |
| ATOM | M 1197 CZ TYR A 153 | 2.00 33,34 |
| ATOM | 1 1198 OH TYR A 153 | 1.00 37.30 |
| ATOM | 1 1199 C TYR A 153 | 1.00 30.10 |
| ATOM | 1 1200 O TYR A 153 | 1.00 32.71 |
| ATOM | 1 1201 N LEU A 154 | |
| ATOM | 1 1202 CA LEU A 154 | 25.05 |
| ATOM | 1 1203 CB LEU A 154 | 1.00 32.87 |
| ATOM | 1204 CG LEU A 154 | 2.00 31.40 |
| MOTA | 1205 CD1 LEU A 154 | 34.910 11.053 126.324 1.00 29.68 35.898 11.953 125.605 1 00 29.20 |
| ATOM | 1206 CD2 LEU A 154 | 1.00 23.23 |
| ATOM | 1207 C LEU A 154 | 34.989 11.278 127.829 1.00 27.19 31.020 10.952 126.232 1.00 34.63 |
| ATOM | 1208 O LEU A 154 | 22 1.00 34.03 |
| MOTA | 1209 N ARG A 155 | 30.475 11.379 127.250 1.00 32.58 |
| MOTA | | 30.443 10.999 125.035 1.00 36.63 |
| ATOM | | 29.107 11.569 124.869 1.00 38.36 |
| ATOM | 1212 CG ARG A 155 | 28.661 11.502 123.405 1.00 36.32 |
| ATOM | 1213 CD ARG A 155 | 29.581 12.253 122.460 1.00 43.15 |
| ATOM | 1214 NE ARG A 155 | 29.100 12.201 121.023 1.00 41.10 27.936 13.047 120.768 1 00 44.00 |
| ATOM | 1215 CZ ARG A 155 | 2,00 44.00 |
| ATOM | 1216 NH1 ARG A 155 | 20 1100 14.00 |
| MOTA | 1217 NH2 ARG A 155 | |
| ATOM | 1218 C ARG A 155 | |
| MOTA | 1219 O ARG A 155 | 1 |
| MOTA | 1220 N LYS A 156 | |
| MOTA | 1221 CA LYS A 156 | |
| MOTA | 1222 CB LYS A 156 | |
| ATOM | 1223 CG LYS A 156 | 2.00 41.00 |
| ATOM | 1224 CD LYS A 156 | 1.00 51.15 |
| ATOM | 1225 CE LYS A 156 | 27.169 7.505 123.781 1.00 55.56 26.117 7.502 122.676 1.00 55.63 |
| ATOM | 1226 NZ LYS A 156 | 24.993 8.425 123.013 1.00 49.15 |
| ATOM | 1227 C LYS A 156 | 27.527 8.932 128.076 1.00 39.91 |
| MOTA | .1228 O LYS A 156 | 26.636 8.658 128.876 1.00 37.01 |
| MOTA | 1229 N LYS A 157 | 28.703 9.431 128.448 1.00 37.73 |
| MOTA | 1230 CA LYS A 157 | 28.985 9.725 129.847 1.00 36.52 |
| ATOM | 1231 CB LYS A 157 | 30.493 9.700 130.122 1.00 35.64 |
| ATOM | 1232 CG LYS A 157 | 31.094 8.308 130.174 1.00 35.44 |
| ATOM | 1233 CD LYS A 157 | 30.509 7.510 131.335 1.00 31.28 |
| ATOM | 1234 CE LYS A 157 | 31.077 6.106 131 388 1 00 31 40 |
| ATOM | 1235 NZ LYS A 157 | 30.464 5.310 132,493 1,00 36 39 |
| ATOM ATOM | 1236 C LYS A 157 | 28.423 11.097 130.197 1 00 30 12 |
| MOTA | | 28.531 11.547 131.336 1.00 37 61 |
| ATOM | | 27.842 11.768 129.205 1 00 36 27 |
| ATOM | | 27.257 13.074 129.452 1.00 34 31 |
| | | 27.972 14.293 128.894 1.00 36 36 |
| MOTA MOTA | 4.7.40 | 27.438 15.399 128.963 1.00 32 96 |
| ATOM | | 29.170 14.117 128.344 1.00 33 89 |
| | | 29.892 15.260 127.796 1.00 30.29 |
| MOTA | | 31.346 14.892 127.504 1.00 28.62 |
| MOTA | | 32.13/ 14.555 128.730 1.00 28.80 |
| ATOM | | 32.043 13.300 129.310 1.00 30.41 |
| ATOM | | 34.951 15.513 129.327 1.00 29.37 |
| ATOM | 1248 CE1 PHE A 159 | 32.749 12.996 130.472 1.00 34.42 |
| MOTA | 1249 CE2 PHE A 159 | 33.661 15.223 130.488 1.00 31.10 |
| MOTA | 1250 CZ PHE A 159 1251 C PHE A 159 | 33.561 13.963 131.062 1.00 32.32 |
| MOTA | | 29.224 15.786 126.536 1.00 28.88 |
| | | 28.765 15.003 125.705 1.00 27.71 |
| | | 29.180 17.110 126.402 1.00 30.20 |
| ATOM | 1254 CA LYS A 160 | 28.550 17.766 125.254 1.00 33.98 |
| | | the state of the s |

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Figure 18-20

| | • | |
|--------|-------------------------------------|---|
| ATO | M 1255 CB LYS A 160 | 27.390 18.653 125 719 1 00 26 26 |
| ATO: | M 1256 CG LYS A 160 | |
| ATO: | X 100 | 20.2/3 17.914 126.419 1 nn 30 40 |
| | 05 SIS A 160 | 25.105 18.850 126.723 1.00 48.58 |
| ATO | CD 513 M 180 | 25 500 00 1.00 48.58 |
| ATO | M 1259 NZ LYS A 160 | 25 024 10 22 22 1.00 50.8 |
| ATO | M 1260 C LYS A 160 | 20 40. |
| ATOI | 15 11 100 | 23.404 18.616 124.394 1.00 32 Ed |
| | | |
| ATO | 101 H 6)4: | 30 700 1.00 30.38 |
| IOTA | M 1263 CA ARG A .161 | 21 22 23 124 867 1.00 31.43 |
| ATON | 1 1264 CB ARG A 161 | |
| ATOM | 12.01 | 31.701 21.048 124.673 1.00 34 45 |
| ATOM | 11/10 W 10T | - 30.476 21.854 124.610 1.00 37.63 |
| | FM A 101 | |
| · ATOM | 1267 NE ARG A 161 | 21 150 |
| ATOM | 1 1268 CZ ARG A 161 | |
| ATOM | 12(0 11 101 | 23.337 127.414 1.00 43 33 |
| ATOM | | 29.117 22.985 127.274 1.00 45.95 |
| | ING A TOT | 30 003 0 |
| ATOM | 1271 C ARG A 161 | 22 000 |
| ATOM | 1272 O ARG A 161 | 77 700 |
| ATOM | 1210 X 101 | 33.732 19.090 125.092 1 nn 20 ca |
| | - 122 A 102 | |
| ATOM | III A 102 | |
| MOTA | 1275 CB ILE A 162 | |
| ATOM | 1276 CG2 TLE A 162 | |
| ATOM | IDE A 102 | 33.407 14.976 122.898 1 00 24 05 |
| - | · · · · · · · · · · · · · · · · · · | 33.147 15.355 123.879 1.00 30.25 |
| MOTA | 1278 CD1 ILE A 162 | 33 564 30.25 |
| MOTA | 1279 C ILE A 162 | 25 252 27 |
| ATOM | 1280 O ILE A 162 | 24 075 25 25 25 25 25 25 25 25 25 25 25 25 25 |
| MOTA | 1281 N LEU A 163 | 34.0/0 1/.9/3 120.762 1.00 27 88 |
| ATOM | | 36.626 18.067 122 160 1 00 03 |
| | | 37.575 18.534 121 156 1 00 25 |
| ATOM | 1283 CB LEU A 163 | 20 20 43.74 |
| ATOM | 1284 CG LEU A 163 | 70 50 |
| ATOM | 1285 CD1 LEU A 163 | 70 010 |
| ATOM | 1286 CD2 LEU A 163 | 39.213 20.591 119.473 1.00 26.25 |
| ATOM | 1200 CD2 LSU A 163 | 40.301 21.252 121 560 1 00 22 26 |
| | 1287 C LEU A 163 | 20 545 45 |
| MOTA | 1288 O LEU A 163 | 20 052 |
| ATOM | 1289 N TYR A 164 | 20 000 |
| ATOM | 1290 CA TYR A 164 | 38.808 17.257 119.496 1.00 26.97 |
| ATOM | | 39.747 16.241 119.010 1 00 26 07 |
| | | 39.021 15.181 118.179 1.00 23.38 |
| ATOM | 1292 CG TYR A 164 | 20 044 |
| ATOM | 1293 CD1 TYR A 164 | 100 21.76 |
| ATOM | 1294 CE1 TYR A 164 | 42 42 22 24 24 24 24 24 24 24 24 24 24 2 |
| ATOM | 1295 CD2 TYR A 164 | 41.419 12.224 117.794 1.00 22.90 |
| MOTA | 11 104 | 40.202 14.142 116.194 1.00 19 74 |
| | | 41.060 13.190 115.616 1.00 23.36 |
| ATOM | 1297 CZ TYR A 164 | 4 |
| ATOM | 1298 OH TYR A 164 | 40 505 |
| MOTA | 1299 C TYR A 164 | 40 700 18.41 |
| MOTA | 11 204 | 40.798 16.923 118.138 1.00 21 67 |
| | | 40.473 .17.511 117 112 1 00 10 75 |
| ATOM | 1301 N ILE A 165 | |
| MOTA | 1302 CA ILE A 165 | 43 440 23.01 |
| ATOM | 1303 CB ILE A 165 | 45 45 45 |
| ATOM | 1304 CG2 TLE A 165 | 15 100 20.41 |
| ATOM | | 45.12/ 19.017 117.937 1.00 19 36 |
| | | 43.035 19.482 119.274 1.00 23.36 |
| ATOM | 1306 CD1 ILE A 165 | 43 605 |
| ATOM | 1307 C ILE A 165 | 14 040 |
| ATOM | 1308 O ILE A 165 | 14 570 |
| ATOM | | 44.338 15.505 117.971 1.00 21 91 |
| | | 44.242 16.408 115.920 1 00 24 20 |
| ATOM | 1310 CA ASP A 166 | 4E 022 |
| ATOM | 1311 CB ASP A 166 | 44 140 |
| ATOM | 1312 CG ASP A 166 | 44 600 |
| | 1313 OD1 ASP A 166 | |
| | | 45.831 13.456 113.068 1 00 30 37 |
| | 1314 OD2 ASP A 166 | 43.995 12.437 113 717 1 00 22 27 |
| | 1315 C ASP A 166 | 16 310 15 004 444 44 |
| MOTA | 1316 O ASP A 166 | 46 705 |
| | 1317 N LEU A 167 | 42 462 |
| | 220 11 20 1 | 47.432 15.597 115.227 1.00 23 43 |
| | 1710 | 48.738 16.068 114.722 1.00 24.67 |
| | 1319 CB LEU A 167 | |
| TOM | 1320 CG LEU A 167 | 10 143 -0.502 125.06/ 1.00 21.90 |
| | | 49.143 17.444 116.858 1.00 26.62 |
| | | · |

| 3 00034 | 1221 | CD1 | | | |
|---------|------|-----------------|---------------------|----------------|------------|
| MOTA | | | 50.249 | 17.845 117.821 | 1.00 25.88 |
| ATOM | 1322 | CD2 LEU A 167 | 48.658 | 18.668 116.092 | |
| ATOM | 1323 | C LEU A 167 | 49.405 | | |
| ATOM | 1324 | O LEU A 167 | | | |
| | | O DEO A 167 | 50.504 | | |
| MOTA | 1325 | N ASP A 168 | 48.736 | 13.977 113.488 | 1.00 24.69 |
| ATOM- | 1326 | CA ASP A 168 | 49.244 | 12.975 112.555 | 1.00 24.59 |
| ATOM | 1327 | CB ASP A 168 | 48.209 | | |
| ATOM | 1328 | | | | |
| | | CG ASP A 168 | 48.722 | 10.669 111.608 | 1.00 28.11 |
| MOTA | 1329 | C ASP A 168 | 49.423 | 13.686 111.209 | 1.00 24.17 |
| ATOM | 1330 | O _ASP A 168 | 48.629 | 14.559 110.865 | |
| ATOM | 1331 | OD1 ASP A 168 | 49.085 | | |
| | | | | | |
| ATOM | 1332 | OD2 ASP A 168 | 48.777 | | |
| MOTA | 1333 | N ALA A 169 | 50.448 | 13.312 110.446 | 1.00 21.29 |
| ATOM | 1334 | CA ALA A 169 | 50.693 | 13.927 109.140 | |
| ATOM | 1335 | CB ALA A 169 | 52.068 | | |
| | | | | 13.498 108.601 | 1.00 21.17 |
| MOTA | 1336 | C ALA A 169 | 49.612 | 13.636 108.093 | 1.00 26.57 |
| MOTA | 1337 | O ALA A 169 | 49.641 | 14.204 107.000 | 1.00 26.90 |
| ATOM | 1338 | N HIS A 170 | 48.673 | 12.746 108.406 | 1.00 21.63 |
| MOTA | 1339 | CA HIS A 170 | 47.592 | | |
| | | | | 12.445 107.468 | 1.00 24.79 |
| ATOM | 1340 | C HIS A 170 | 46.243 | 12.867 108.045 | 1.00 20.98 |
| ATOM | 1341 | O HIS A 170 | 46.044 | 12.849 109.255 | 1.00 24.12 |
| ATOM | 1342 | CB HIS A 170 | 47.550 | 10.950 107.131 | 1.00 23.17 |
| MOTA | 1343 | CG HIS A 170 | | | |
| | | | 48.830 | | 1.00 30.28 |
| ATOM | 1344 | ND1 HIS A 170 | 49.842 | 9.982 107.385 | 1.00 31.00 |
| MOTA | 1345 | CE1 HIS A 170 | 50.825 | 9.634 106.577 | 1.00 24.33 |
| MOTA | 1346 | CD2 HIS A 170 | 49.224 | 10.329 105.273 | 1.00 22.88 |
| ATOM | 1347 | NE2 HIS A 170 | 50.502 | 9.828 105.285 | |
| | 1348 | | | | 1.00 21.89 |
| MOTA | | N HIS A 171 | 45.317 | 13.231 107.171 | 1.00 21.14 |
| ATOM | 1349 | CA HIS A 171 | 43.993 | 13.661 107.591 | 1.00 25.57 |
| MOTA | 1350 | CB HIS A 171 | 43.234 | 14.242 106.404 | 1.00 22.47 |
| MOTA | 1351 | CG HIS A 171 | 41.857 | 14.719 106.746 | 1.00 29.75 |
| ATOM | 1352 | CD2 HIS A 171 | | | |
| | | | 41.433 | 15.648 107.634 | 1.00 25.58 |
| MOTA | 1353 | ND1 HIS A 171 | 40.721 | 14.201 106.160 | 1.00 28.90 |
| ATOM | 1354 | CE1 HIS A 171 . | 39.656 | 14.787 106.676 | 1.00 25.35 |
| MOTA | 1355 | NE2 HIS A 171 | 40.060 | 15.669 107.573 | 1.00 32.40 |
| ATOM | 1356 | C HIS A 171 | | | |
| | | | 43.169 | 12.533 108.204 | 1.00 29.61 |
| MOTA | 1357 | O HIS A 171 | 43.169 | 11.411 107.698 | 1.00 27.62 |
| ATOM | 1358 | N CYS A 172 | 42.461 | 12.852 109.286 | 1.00 26.52 |
| ATOM | 1359 | CA CYS A 172 | 41.610 | 11.897 109.987 | 1.00 24.82 |
| ATOM | 1360 | CB CYS A 172 | 41.460 | 12.322 111.456 | 1.00 29.47 |
| | 1361 | SG CYS A 172 | | | |
| ATOM | | | 40.959 | 14.065 111.717 | 1.00 25.69 |
| ATOM | 1362 | C CYS A 172 | 40.237 | 11.797 109.314 | 1.00 28.21 |
| ATOM | 1363 | O CYS A 172 | 39.211 | 12.131 109.914 | 1.00 26.78 |
| ATOM | 1364 | N ASP A 173 | 40.213 | 11.332 108.066 | 1.00 22.05 |
| ATOM | 1365 | CA ASP A 173 | | | |
| | | CD 10D 1 100 | 38.949 | 11.217 107.350 | 1.00 27.39 |
| ATOM | 1366 | CB ASP A 173 | 39.167 | 10.646 105.931 | 1.00 30.47 |
| MOTA | 1367 | CG ASP A 173 | 39.824 ⁻ | 9.264 105.922 | 1.00 29.77 |
| ATOM | 1368 | OD1 ASP A 173 | 39.886 | 8.658 104.830 | 1.00 21.14 |
| ATOM | | OD2 ASP A 173 | 40.288 | | |
| | | | | 8.787 106.978 | 1.00 30.04 |
| ATOM | | C ASP A 173 | 37.895 | 10.400 108.105 | 1.00 27.86 |
| MOTA | 1371 | O ASP A 173 | 36.720 | 10.762 108.120 | 1.00 23.47 |
| ATOM | 1372 | N GLY A 174 | 38.309 | .9.315 108.753 | 1.00 25.84 |
| ATOM | | CA GLY A 174 | 37.344 | | |
| | | | | | 1.00 28.49 |
| MOTA | | C GLY A 174 | 36.694 | 9.296 110.619 | 1.00 26.14 |
| MOTA | 1375 | O GLY A 174 | 35.475 | 9.287 110.780 | 1.00 21.39 |
| ATOM | 1376 | N VAL A 175 | 37.510 | 9.984 111.409 | 1.00 27.24 |
| | | CA VAL A 175 | | | |
| ATOM | | | 36.995 | 10.773 112.523 | 1.00 25.53 |
| ATOM | | CB VAL A 175 | . 38.137 | 11.299 113.401 | 1.00 30.54 |
| ATOM | 1379 | CG1 VAL A 175 | 37.565 | 12.105 114.566 | 1.00 28.02 |
| ATOM | | CG2 VAL A 175 | 38.973 | 10.129 113.911 | 1.00 21.30 |
| | | VAL A 175 | | | *** |
| MOTA | | | 36.163 | 11.955 112.035 | 1.00 25.01 |
| ATOM | | VAL A 175 | 35.130 | 12.282 112.623 | 1.00 21.60 |
| ATOM | 1383 | V GLN A 176 | 36.601 | 12.594 110.957 | 1.00 25.43 |
| ATOM | | CA GLN A 176 | 35.854 | 13.730 110.426 | 1.00 26.12 |
| | | CB GLN A 176 | | 14.336 109.205 | |
| ATOM | | - | 36.554 | 14.330 100.405 | 1.00 24.71 |
| ATOM | 1386 | CG GLN A 176 | 35.682 | 15.349 108.469 | 1.00 26.68 |

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Figure 18-22

| ATO: | M 1387 CD GLN A 176 | 36.385 16.002 107.306 1.00 29 54 |
|--------|----------------------|---|
| ATO | | 20 25.54 |
| | | 37.382 16.704 107.486 1.00 26.93 |
| ATO | | 35.872 15.776 106.099 1.00 27.58 |
| ATO | M 1390 C GLN A 176 | 34.446 13.316 110.029 1.00 27.63 |
| ATOI | M 1391 O GLN A 176 | 33.481 14.021 110.319 1.00 25.93 |
| ATO | | 2.00 23.33 |
| ATOI | , | |
| | M 1394 CB GLU A 177 | 33.027 11.696 108.915 1.00 32.72 |
| OTA | | 33.181 10.445 108.053 1.00 34.20 |
| ATON | | 31.905 10.069 107.329 1.00 39.40 |
| OTA | 1 1396 CD GLU A 177 | 32.060 8.819 106.497 1.00 41.42 |
| ATOL | | |
| ATOM | 1 1398 OE2 GLU A 177 | |
| ATOM | | |
| | | 32.128 11.377 110.099 1.00 30.54 |
| ATOM | | 30.945 11.697 110.093 1.00 25.39 |
| ATOM | | 32.707 10.750 111.114 1.00 27.03 |
| MOTA | 1 1402 CA ALA A 178 | 31.971 10.365 112.303 1.00 30.67 |
| ATOM | | 2.00 30.07 |
| ATOM | | 2.00 50,45 |
| | | 31.261 11.519 113.003 1.00 33.21 |
| MOTA | | 30.145 11.355 113.493 1.00 28.64 |
| ATOM | | 31.888 12.688 113.055 1.00 29.27 |
| ATOM | 1407 CA PHE A 179 | 31.256 13.801 113.751 1.00 30.49 |
| ATOM | | |
| ATOM | | |
| MOTA | 1410 CD1 PHE A 179 | 32.469 12.909 115.781 1.00 24.43 |
| | | 33.749 12.375 115.657 1.00 25.04 |
| . ATOM | | 31.536 12.233 116.563 1.00 23.09 |
| ATOM | | 34.103 11.184 116.293 1.00 16 56 |
| MOTA | 1413 CE2 PHE A 179 | 31.881 11.038 117.204 1.00 26.38 |
| ATOM | 1414 CZ PHE A 179 | |
| ATOM | 1415 C PHE A 179 | |
| ATOM | 1416 O PHE A 179 | |
| | | 31.006 16.152 113.399 1.00 31.32 |
| MOTA | 1417 N TYR A 180 | 30.980 14.828 111.584 1.00 31.68 |
| ATOM | 1418 CA TYR A 180 | 30.829 15.925 110.646 1.00 32.76 |
| ATOM | 1419 CB TYR A 180 | 30.931 15.378 109.213 1.00 35.12 |
| MOTA | 1420 CG TYR A 180 | 31.331 16:406 108.172 1.00 36.27 |
| ATOM | 1421 CD1 TYR A 180 | |
| ATOM | 1422 CE1 TYR A 180 | |
| ATOM | | 30.801 17.791 106.244 1.00 34.81 |
| | | 32.624 16.937 108.154 1.00 36.32 |
| MOTA | 1424 CE2 TYR A 180 | 33.007 17.879 107.203 1.00 37.83 |
| ATOM | 1425 CZ TYR A 180 | 32.088 18.304 106.250 1.00 36.05 |
| ATOM | 1426 OH TYR A 180 | 32.446 19.255 105.323 1.00 28.04 |
| ATOM | 1427 C TYR A 180 | 29.518 16.696 110.825 1.00 30.94 |
| ATOM | 1428 O TYR A 180 | 00 450 45 55 55 |
| ATOM | 1429 N ASP A 181 | 20 172 17 204 114 |
| | | 28.473 16.026 111.299 1.00 31.56 |
| ATOM | | 27.180 16.691 111.444 1.00 37.30 |
| ATOM | 1431 CB ASP A 181 | 26.086 15.833 110.807 1.00 37.68 |
| ATOM | 1432 CG ASP A 181 | 25.645 14.689 111.705 1.00 39.86 |
| ATOM | 1433 OD1 ASP A 181 | 26.505 13.963 112.233 1.00 43.25 |
| MOTA | 1434 OD2 ASP A 181 | |
| ATOM | 1435 C ASP A 181 | |
| ATOM | 1436 O ASP A 181 | 2.00 30.01 |
| | | |
| ATOM | 1437 N THR A 182 | 27.689 17.066 113.810 1.00 40.86 |
| atom | 1438 CA THR A 182 | 27.327 17.412 115.184 1.00 38.27 |
| ATOM | 1439 CB THR A 182 | 27.433 16.201 116.133 1.00 37.99 |
| ATOM | 1440 OG1 THR A 182 | |
| ATOM | 1441 CG2 THR A 182 | 20 000 15 001 |
| ATOM | | 20 177 |
| | | 28.177 18.546 115.746 1.00 39.51 |
| ATOM | 1443 O THR A 182 | 29.365 18.673 115.433 1.00 40.07 |
| ATOM | 1444 N ASP A 183 | 27.557 19.369 116.582 1.00 37.01 |
| ATÓM | 1445 CA ASP A 183 | 28.250 20.497 117.181 1.00 37.74 |
| ATOM | 1446 CB ASP A 183 | 2 |
| ATOM | 1447 CG ASP A 183 | 25 136 |
| | | 26.136 21.493 118.155 1.00 38.01 |
| atom | 1448 OD1 ASP A 183 | 25.614 20.357 118.210 1.00 34.94 |
| atom | 1449 OD2 ASP A 183 | 25.720 22.470 118.814 1.00 38.17 |
| ATCM · | 1450 C ASP A 183 | 28.762 20.161 118.578 1.00 35.27 |
| ATCM | 1451 O ASP A 183 | 29.337 21.015 119.251 1.00 35.16 |
| ATOM | 1452 N GLN A 184 | 20 560 |
| | | 28.562 18.917 119.012 1.00 35.10 |

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| ATOM | 1453 | CA | GLN A | 184 | 29.030 | 18.505 | 120.333 | 1.00 | 35.16 |
|--------------|--------------|------------|-------|-----|------------------|------------------|--------------------|------|----------------|
| ATOM | 1454 | CB | GLN A | | 28.155 | 17.382 | 120.906 | 1.00 | 36.94 |
| ATOM | 1455 | CG | GLN A | 184 | 26.663 | | 120.988 | | 38.34 |
| MOTA | 1456 | CD | GLN A | 184 | 25.881 | | 121.838 | | 43.68 |
| ATOM | 1457 | OE1 | GLN A | 184 | 26.027 | | 121.696 | | 35.48 |
| ATOM | 1458 | NE2 | GLN A | | 25.036 | | 122.723 | | 51.06 |
| ATOM | 1459 | С | GLN A | 184 | 30.479 | | 120.253 | | 36.32 |
| MOTA | 1460 | 0 | GLN A | | 31.135 | | 121.275 | | 34.24 |
| MOTA | 1461 | N | VAL A | | 30.976 | | 119.028 | | 34.51 |
| ATOM | 1462 | CA | VAL A | | 32.348 | 17.443 | 118.804 | 1.00 | |
| MOTA | 1463 | CB | VAL A | | 32.393 | | 118.259 | | 35.11 23.80 |
| MOTA | 1464 | CG1 | VAL A | | 33.834 | 15.567 | 118.003 119.242 | | 26.00 |
| ATOM | 1465 | CG2 | VAL A | | 31.731 | | | | 33.11 |
| ATOM | 1466 | C | VAL A | | 33.053 | | 117.803 116.714 | | 27.73 |
| ATOM | 1467 | 0 | VAL A | | 32.545 34.215 | | 118.184 | | 31.49 |
| ATOM | 1468 | N | PHE A | | 34.213 | | 117.291 | | 30.63 |
| MOTA | 1469 | CA CB | PHE A | | 35.420 | | 117.991 | | 30.34 |
| ATOM | 1470 1471 | CG | PHE A | | 36.008 | | 117.051 | | 30.22 |
| ATOM | 1472 | CD1 | PHE A | | 35.265 | | 116.656 | | 32.23 |
| MOTA MOTA | 1473 | CD2 | PHE A | | 37.284 | | 116.524 | 1.00 | 29.37 |
| ATOM | 1474 | CE1 | PHE A | | 35.785 | | 115.748 | 1.00 | 27.87 |
| ATOM | 1475 | CE2 | PHE A | | 37.813 | 22.794 | 115.615 | 1.00 | 28.54 |
| ATOM | 1476 | CZ | PHE A | | 37.064 | | 115.227 | | 30.80 |
| ATOM | 1477 | С | PHE A | 186 | 36.232 | | 116.879 | | 33.38 |
| ATOM | 1478 | 0 | PHE A | | 36.952 | 18.426 | 117.729 | | 28.30 |
| ATOM | 1479 | N | VAL A | | 36.478 | | 115.574 | | 32.00 |
| MOTA | 1480 | CA | VAL A | | 37.645 | | 115.060 | | 29.70 |
| MOTA | 1481 | CB | VAL A | | 37.252 | 17.095 | 114.019 113.405 | | 27.77 |
| ATOM | 1482 | CG1 | VAL A | | 38.510 36.410 | 16.400 | 114.672 | | 25.98 |
| MOTA | 1483 | CG2 | VAL A | | 38.604 | 10.003 | 114.392 | | 31.03 |
| MOTA | 1484 1485 | С 0 | VAL A | | 38.215 | 19 895 | 113.491 | | 31.88 |
| MOTA | 1486 | N | LEU A | | 39.850 | | 114.857 | | 24.88 |
| ATOM ATOM | 1487 | CA | LEU A | | 40.899 | | 114.304 | 1.00 | 26.92 |
| ATOM | 1488 | CB | LEU A | | 41.468 | | 115.361 | | 27.04 |
| ATOM | 1489 | CG | LEU A | | 42.823 | | 114.963 | | 25.15 |
| ATOM | 1490 | CD1 | LEU A | 188 | 42.686 | | 113.648 | | 18.53 |
| ATOM | 1491 | CD2 | LEU A | 188 | 43.330 | 22.485 | 116.068 | | 28.81 |
| MOTA | 1492 | С | LEU A | | 42.022 | | 113.815 | | 31.22 |
| ATOM | 1493 | 0 | LEU A | | 42.579 | 18.333 | | | 25.83 30.53 |
| ATOM | 1494 | N | SER A | | 42.369 | 19.230 | 112.540 112.007 | | 30.13 |
| ATOM | 1495 | CA | SER A | | 43.429 42.821 | 17 240 | 111.199 | | 33.41 |
| MOTA | 1496 | CB | SER A | | 43.837 | 16.474 | | | 32.98 |
| MOTA | 1497 1498 | OG C | SER A | | 44.448 | | 111.143 | | 27.94 |
| MOTA | 1499 | ō | SER A | | 44.084 | 19.891 | 11 1.253 | 1.00 | 22.14 |
| ATOM ATOM | 1500 | N | LEU A | | 45.728 | 18.877 | | 1.00 | 24.80 |
| MOTA | 1501 | CA | LEU A | | 46.805 | 19.438 | 110.614 | 1.00 | 22.23 |
| ATOM | | CB | LEU A | | 47.955 | | 111.459 | | 23.69 |
| MOTA | 1503 | CG | LEU A | 190 | 47.733 | | 112.522 | | 28.92 |
| ATOM | 1504 | CD1 | LEU A | 190 | 49.070 | 21.780 | 112.740 | | 23.01 |
| ATOM | 1505 | CD2 | LEU A | 190 | 46.691 | 22.093 | 112.087 | | 28.11 |
| MOTA | 1506 | С | LEU A | | 47.300 | 18.210 | 109.872 | | 22.69 |
| MOTA | 1507 | 0 | LEU A | | 47.416 | | 110.465 | | 16.55 19.22 |
| ATOM | 1508 | N | HIS A | | 47.599 | 18.353 | | | 23.28 |
| MOTA | 1509 | CA | HIS A | | 48.046 46.870 | 17.210 | | | 15.58 |
| atom | 1510 | CB | HIS A | | | 16.242 16.915 | 107.256 | | 24.16 |
| MOTA | 1511 | CG | HIS A | 191 | 45.591 45.034 | 17 174 | 106.038 | | 17.71 |
| ĄŢOM | 1512 | CDZ ND1 | HIS A | 191 | 44.695 | 17.124 | | | 23.76 |
| MOTA | 1513 | CE1 | HIS A | 191 | 43.644 | 17.913 | 107.545 | 1.00 | 19.78 |
| MOTA | 1514 1515 | MES. | HIS A | 191 | 43.823 | 17.746 | 106.246 | 1.00 | 27.87 |
| ATOM | 1515 | C | HIS A | 191 | 48.570 | 17.620 | 106.434 | 1.00 | 23.65 |
| ATCM | 1517 | Ö | HIS A | 191 | 48.419 | 18.761 | 106.017 | 1.00 | 23.89 |
| ATOM ATOM | 1518 | N | GLN A | 192 | 49.209 | 16.681 | 105.746 | 1.00 | 23.49 |
| 2 | | | | | | | | | |

| | | | | | • | | | | |
|--------|-------|------|-------|-------|---|--------|--------|---------|------------|
| ATOM | 1519 | CA | GLN A | 192 | | 49.718 | 16.950 | 104.412 | 1.00 20.55 |
| ATOM | 1520 | CB | GLN A | 192 | | 50.474 | 15.738 | 103.864 | 1.00 23.63 |
| | 1521 | CG | GLN A | | | 51.528 | 15.181 | 104.797 | 1.00 24.07 |
| ATOM | | | | | | 52.110 | | 104.293 | 1.00 26.90 |
| MOTA | 1522 | CD | GLN A | | | | | 103.421 | 1.00 20.21 |
| MOTA | 1523 | OE1 | GLN A | | | 52.986 | | | |
| ATOM | 1524 | NE2 | GLN A | 192 | | 51.605 | | 104.828 | 1.00 23.52 |
| MOTA | 1525 | С | GLN A | 192 | | 48.478 | 17.174 | 103.570 | 1.00 21.41 |
| | 1526 | ō | GLN A | | | 47.478 | 16.466 | 103.726 | 1.00 20.15 |
| MOTA | | | | 193 | | 48.528 | 18.167 | 102.692 | 1.00 24.36 |
| MOTA | 1527 | N | | | | 47.397 | | 101.821 | 1.00 23.98 |
| MOTA | 1528 | CA | SER A | | | | | 100.820 | 1.00 24.60 |
| MOTA | 1529 | CB | | 193 | • | 47.760 | | | |
| ATOM | 1530 | OG | SER A | 193 | | 46.729 | 19.660 | 99.861 | 1.00 25.83 |
| ATOM | 1531 | С | SER A | 193 | | 46.985 | | 101.045 | 1.00 23.74 |
| MOTA | 1532 | 0 | SER A | 1.193 | | 47.829 | 16.492 | 100.506 | 1.00 19.80 |
| | 1533 | N· | PRO A | | | 45.674 | 16.936 | 100.953 | 1.00 24.85 |
| ATOM | 1534 | CD | PRO 7 | | | 44.561 | 17.719 | 101.507 | 1.00 25.08 |
| MOTA | | | PRO P | | | 45.151 | | 100.235 | 1.00 29.25 |
| MOTA | 1535 | CA | | | | | | 100.444 | 1.00 30.51 |
| MOTA | 1536 | CB | PRO A | | | 43.641 | 20.301 | 100.933 | 1.00 30.21 |
| MOTA | 1537 | CG | PRO A | | | 43.554 | | 101.758 | |
| ATOM | 1538 | С | PRO A | 194 | | 45.527 | 15.825 | 98.756 | 1.00 30.75 |
| ATOM | 1539 | . 0 | PRO A | 194 | | 45.420 | 14.830 | 98.041 | 1.00 30.04 |
| ATOM | 1540 | N | GLU A | | | 45.967 | 16.991 | 98.298 | 1.00 26.28 |
| | 1541 | CA | GLU A | | | 46.343 | 17.127 | 96.898 | 1.00 31.11 |
| MOTA | | | GLU A | | | 46.738 | 18.570 | 96.571 | 1.00 29.52 |
| MOTA | 1542 | CB | | | | 45.680 | 19.600 | 96.933 | 1.00 38.32 |
| MOTA | 1543 | CG | GLU A | | | 45.976 | 20.972 | 96.352 | 1.00 44.15 |
| MOTA | 1544 | CD | GLU A | | | | | 96.434 | 1.00 44.23 |
| MOTA | 1545 | OE1 | | | | 47.139 | 21.425 | | |
| ATOM | 1546 | OE2 | GLU A | 195 | | 45.037 | 21.605 | 95.825 | 1.00 45.06 |
| ATOM | 1547 | С | GLU A | 195 | | 47.499 | 16.193 | 96.552 | 1.00 30.81 |
| ATOM | 1548 | 0 | GLU A | 195 | | 47.582 | 15.705 | 95.426 | 1.00 37.17 |
| ATOM | 1549 | N | TYR A | | | 48.377 | 15.922 | 97.515 | 1.00 25.01 |
| | 1550 | CA | TYR A | | | 49.517 | 15.053 | 97.242 | 1.00 23.43 |
| ATOM | | | TYR A | | | 50.810 | 15.881 | 97.223 | 1.00 26.67 |
| MOTA | 1551 | CB | | | | 51.255 | 16.424 | 98.572 | 1.00 26.78 |
| ATOM | 1552 | CG | | 196 | | | 15.625 | 99.476 | 1.00 26.08 |
| MOTA | 1553 | | TYR A | | | 51.957 | | 100.734 | 1.00 26.77 |
| ATOM | 1554 | CEi | TYR A | | | 52.338 | | | |
| ATOM | 1555 | CD2 | TYR A | | • | 50.944 | 17.731 | 98.958 | 1.00 27.55 |
| ATOM | 1556 | CE2 | TYR A | 196 | | 51.320 | 18.226 | 100.216 | 1.00 25.95 |
| ATOM | 1557 | CZ | TYR A | 196 | | 52.012 | | 101.096 | 1.00 24.78 |
| ATOM | 1558 | · OH | TYR A | | | 52.356 | 17.879 | 102.345 | 1.00 25.50 |
| | 1559 | c. | TYR A | | | 49.670 | 13.906 | 98.229 | 1.00 27.05 |
| ATOM | 1560 | o . | TYR ? | | | 50.585 | 13.088 | 98.096 | 1.00 24.02 |
| MOTA | | | ALA A | | | 48.785 | 13.822 | 99.214 | 1.00 22.10 |
| ATOM | 1561 | N | | | | 48.928 | 12 760 | 100.199 | 1.00 24.90 |
| ATOM | 1562 | CA | ALA A | | | | 12.700 | 101.437 | 1.00 27.83 |
| ATOM . | 1563 | CB | ALA A | | | 49.627 | | | 1.00 26.20 |
| MOTA | 1554 | С | ALA A | | | 47.644 | | 100.608 | |
| ATOM | 1: 65 | 0 | ALA A | 197 | | 46.553 | | 100.484 | 1.00 22.82 |
| ATOM | 1556 | N | PHE A | 198 | | 47.795 | 10.849 | 101.102 | 1.00 31.74 |
| ATOM | 1567 | CA | PHE A | 198 | | 46.663 | 10.072 | 101.580 | 1.00 28.74 |
| ATOM | 1568 | СВ | PHE A | 198 | | 47.130 | 8.691 | 102.036 | 1.00 30.66 |
| | 1569 | CG | PHE A | | | 46.009 | 7.766 | 102.399 | 1.00 29.61 |
| MOTA | 1570 | | PHE A | | | 45.496 | 6.879 | 101.463 | 1.00 28.76 |
| ATOM | | CDI | DUE 3 | 100 | | 45.426 | 7 822 | 103.657 | 1.00 28.43 |
| MOTA | 1571 | CDZ | PHE A | 100 | | | 6 057 | 101.773 | 1.00 35.72 |
| MOTA | 1572 | CEl | PHE A | 7 TAR | | 44.415 | 1.00 | 102.773 | 1.00 34.62 |
| ATOM | 1573 | CE2 | PHE A | 198 | | 44.340 | 7.004 | 103.970 | 1.00 35 33 |
| ATOM | 1574 | CZ | PHE A | 198 | | 43.837 | | 103.029 | 1.00 35.73 |
| ATOM | 1575 | С | PHE A | 198 | | 46.121 | | 102.802 | 1.00 28.95 |
| | 1576 | ō | PHE A | 198 | | 46.892 | 11.347 | 103.596 | 1.00 25.72 |
| MOTA | 1577 | N | PRO A | | | 44.792 | 10.905 | 102.941 | 1.00 28.27 |
| ATOM | | | PRO A | 199 | | 44.100 | 11.499 | 104.099 | 1.00 33.97 |
| ATOM | 1578 | CD | FRU A | 100 | | 43.813 | 10 364 | 102.008 | 1.00 32.80 |
| ATOM | 1579 | CA | FRO A | | | | 10.304 | 102.858 | 1.00-29.84 |
| ATOM | 1580 | CB | PRO A | | | 42.550 | 10.314 | 102.000 | 1.00 37.32 |
| ATOM | 1581 | CG | PRO A | | | 42.665 | 11.612 | 103.592 | 1.00 37.32 |
| ATOM | 1582 | С | PRO A | 199 | | 43.773 | 11.476 | 100.965 | 1.00 33.02 |
| ATOM | 1583 | 0 | PRO A | 199 | | 44.052 | | 101.280 | 1.00 48.84 |
| | 1584 | N | PHE A | | | 43.441 | 11.156 | 99.734 | 1.00 33.64 |
| MOTA | | | | | | | | | |

141/263 Figure 18-25

| MOTA | 1585 | CA PHE A 200 | 43.418 | 12.179 98.718 | 1.00 28.12 |
|------|------|---------------|----------|----------------|------------|
| MOTA | 1586 | CB PHE A 200 | 43.927 | 11.579 97.411 | 1.00 26.69 |
| | | | | | |
| ATOM | 1587 | | 45.226 | 10.833 97.561 | 1.00 27.33 |
| MOTA | 1588 | CD1 PHE A 200 | 45.239 | 9.510 97.995 | 1.00 29.79 |
| ATOM | 1589 | | 46.439 | 11.461 97.302 | 1.00 24.38 |
| | | | | | |
| MOTA | 1590 | | 46.444 | 8.820 98.168 | 1.00 29.45 |
| ATOM | 1591 | CE2 PHE A 200 | 47.651 | 10.782 97.473 | 1.00 31.41 |
| MOTA | 1592 | CZ PHE A 200 | 47.653 | 9.458 97.906 | 1.00 29.64 |
| | | | | | |
| MOTĄ | 1593 | | 42.042 | 12.795 98.518 | 1.00 26.15 |
| ATOM | 1594 | O _ PHE A 200 | 41.935 | 13.889 97.986 | 1.00 27.96 |
| ATOM | 1595 | N GLU A 201 | 41.002 | 12.101 98.979 | 1.00 28.52 |
| | 1596 | | | | |
| ATOM | | | 39.614 | | 1.00 35.04 |
| ATOM | 1597 | CB GLU A 201 | 38.695 | 11.316 98.819 | 1.00 33.61 |
| ATOM | 1598 | CG GLU A 201 | 39.087 | 10.240 97.838 | 1.00 37.80 |
| ATOM | 1599 | CD GLU A 201 | 38.222 | 9.016 97.997 | 1.00 43.48 |
| | | | | | |
| ATOM | 1600 | OE1 GLU A 201 | 36.992 | 9.142 97.825 | 1.00 40.96 |
| MOTA | 1601 | OE2 GLU A 201 | 38.772 | 7.937 98.298 | 1.00 44.17 |
| ATOM | 1602 | C GLU A 201 | 39.077 | 13.516 99.837 | 1.00 36.30 |
| | | | 20 007 | | |
| MOTA | 1603 | 0 GLU A 201 | . 38.087 | 14.206 99.592 | 1.00 36.47 |
| MOTA | 1604 | N LYS A 202 | 39.693 | 13.552 101.007 | 1.00 34.63 |
| MOTA | 1605 | CA LYS A 202 | 39.229 | 14.460 102.030 | 1.00 34.09 |
| | | CB LYS A 202 | 38.294 | 13.729 102.992 | 1.00 40.88 |
| ATOM | 1606 | | | | |
| MOTA | 1607 | CG LYS A 202 | 37.011 | 13.318 102.292 | 1.00 43.17 |
| ATOM | 1608 | CD LYS A 202 | 35.935 | 12.854 103.230 | 1.00 47.39 |
| ATOM | 1609 | CE LYS A 202 | 34.628 | 12.663 102.469 | 1.00 47.74 |
| | | | | | |
| MOTA | 1610 | | 33.504 | 12.290 103.378 | 1.00 53.56 |
| ATOM | 1611 | C LYS A 202 | 40.382 | 15.101 102.753 | 1.00 36.27 |
| ATOM | 1612 | O LYS A 202 | 41.520 | 14.666 102.613 | 1.00 28.06 |
| ATOM | 1613 | N GLY A 203 | 40.080 | 16.152 103.509 | 1.00 31.91 |
| | | | | | |
| MOTA | 1614 | CA GLY A 203 | 41.115 | 16.862 104.228 | 1.00 33.75 |
| ATOM | 1615 | C GLY A 203 | 41.288 | 18.288 103.729 | 1.00 30.54 |
| ATOM | 1616 | O GLY A 203 | 42.174 | 18.996 104.200 | 1.00 28.04 |
| | 1617 | N PHE A 204 | 40.458 | 18.713 102.778 | 1.00 29.93 |
| ATOM | | | | | |
| MOTA | 1618 | CA PHE A 204 | 40.557 | 20.077 102.260 | 1.00 35.76 |
| ATOM | 1619 | CB PHE A 204 | 39.863 | 20.217 100.901 | 1.00 31.41 |
| ATOM | 1620 | CG PHE A 204 | 40.498 | 19.416 99.803 | 1.00 31.06 |
| | 1621 | CD1 PHE A 204 | 40.169 | 18.075 99.618 | 1.00 35.66 |
| ATOM | | | | | |
| ATOM | 1622 | CD2 PHE A 204 | 41.431 | 20.002 98.955 | 1.00 30.79 |
| MOTA | 1623 | CE1 PHE A 204 | 40.761 | 17.329 98.597 | 1.00 35.20 |
| MOTA | 1624 | CE2 PHE A 204 | 42.033 | 19.267 97.931 | 1.00 36.08 |
| | | CZ PHE A 204 | 41.697 | 17.928 97.751 | 1.00 36.54 |
| ATOM | 1625 | | | | |
| ATOM | 1626 | C PHE A 204 | 39.967 | 21.103 103.231 | 1.00 37.30 |
| ATOM | 1627 | O PHE A 204 | 39.088 | 20.786 104.040 | 1.00 33.56 |
| MOTA | 1628 | N LEU A 205 | 40.451 | 22.337 103.128 | 1.00 38.52 |
| | 1629 | CA LEU A 205 | 40.012 | 23.427 103.993 | 1.00 36.81 |
| ATOM | | | | | |
| ATOM | 1630 | CB LEU A 205 | 40.801 | 24.695 103.659 | 1.00 34.73 |
| ATOM | 1631 | CG LEU A 205 | 40.496 | 25.954 104.479 | 1.00 40.98 |
| MOTA | 1632 | CD1 LEU A 205 | -40.690 | 25.677 105.965 | 1.00 39.87 |
| | 1633 | CD2 LEU A 205 | 41.415 | 27.079 104.032 | 1.00 39.94 |
| ATOM | | | | | |
| ATOM | 1634 | C LEU A 205 | 38.520 | 23.728 103.925 | 1.00 36.58 |
| MOTA | 1635 | O LEU A 205 | 37.931 | 24.178 104.905 | 1.00 40.98 |
| ATOM | 1636 | N GLU A 206 | 37.909 | 23.477 102.774 | 1.00 36.07 |
| | | | | | |
| MOTA | 1637 | CA GLU A 206 | 36.486 | 23.748 102.586 | 1.00 36.30 |
| ATOM | 1638 | CB GLU A 206 | 36.107 | 23.597 101.105 | 1.00 39.98 |
| MOTA | 1639 | CG GLU A 206 | 36.890 | 24.473 100.131 | 1.00 48.04 |
| | 1640 | CD GLU A 206 | 38.307 | 23.980 99.868 | 1.00 51.87 |
| MOTA | | | | | 1.00 50.32 |
| MOTA | 1641 | OE1 GLU A 206 | 39.146 | 23.993 100.792 | |
| ATOM | 1642 | OE2 GLU A 206 | 38.581 | 23.569 98.716 | 1.00 56.69 |
| ATOM | 1643 | C GLU A 206 | 35.572 | 22.852 103.427 | 1.00 33.85 |
| | 1644 | 3 GLU A 206 | 34.433 | 23.213 103.718 | 1.00 26.22 |
| MOTA | | | | | |
| ATOM | 1645 | N GLU A 207 | 36.071 | 21.679 103.805 | 1.00 31.68 |
| ATOM | 1646 | CA GLU A 207 | 35.297 | 20.726 104.599 | 1.00 31.65 |
| ATOM | 1647 | CB GLU A 207 | 36.000 | 19.369 104.566 | 1.00 34.15 |
| | | CG GLU A 207 | 36.044 | 18.741 103.179 | 1.00 33.80 |
| ATOM | 1648 | | | | |
| ATOM | 1649 | CD GLU A 207 | 37.182 | 17.751 103.022 | 1.00 33.85 |
| ATOM | 1650 | OE1 GLU A 207 | 37.487 | 17.025 103.995 | 1.00 33.22 |
| | | | | | |

| ATOM | 1651 OE2 GLU A 207 | 37.760 | 17.688 101.916 | 5 1 00 35 40 |
|------|---------------------|-----------|----------------------------|--------------|
| ATOM | | 35.182 | | |
| ATOM | | | 21.229 106.033 | |
| | | 36.009 | 20.894 106.887 | |
| ATOM | | 34.150 | 22.024 106.302 | 2 1.00 35.99 |
| MOTA | | 33.968 | 22.604 107.634 | 1.00 38.96 |
| MOTA | 1656 CB ILE A 208 | 33.737 | 24.134 107.529 | 1.00 42.74 |
| ATOM | | 33.717 | 24.762 108.914 | 1 00 40 00 |
| ATOM | | | | |
| | 1659 CD1 ILE A 208 | 34.841 | 24.795 106.700 | |
| MOTA | | 36.207 | 24.758 107.335 | |
| ATOM | | 32.821 | 21.998 108.452 | 1.00 38.32 |
| ATOM | 1661 O ILE A 208 | | 22.434 109.571 | |
| ATOM | 1662 N GLY A 209 | 32.142 | 20.997 107.901 | 1.00 34.36 |
| ATOM | 1663 CA GLY A 209 | | | |
| ATOM | 1664 C GLY A 209 | | 20.374 108.620 | |
| | | | 20.673 107.993 | |
| MOTA | 1665 O GLY A 209 | 29.579 | 21.581 107.173 | 1.00 40.56 |
| ATOM | 1666 N GLU A 210 | 28.676 | 19.917 108.38 0 | 1.00 37.38 |
| ATOM | 1667 CA GLU A 210 | | 20.118 107.831 | 1.00 42.34 |
| MOTA | 1668 CB GLU A 210 | 27.008 | 19.012 106.823 | |
| ATOM | 1669 CG GLU A 210 | | | |
| | | | 17.636 107.460 | |
| ATOM | | | 16.532 106.443 | |
| MOTA | 1671 OE1 GLU A 210 | 26.385 | 15.379 106.860 | 1.00 50.59 |
| MOTA | 1672 OE2 GLU A 210 | | 16.810 105.226 | 1.00 53.78 |
| MOTA | 1673 C GLU A 210 | | 20.114 108.938 | 1.00 42.90 |
| ATOM | 1674 O GLU A 210 | | | |
| ATOM | 1675 N GLY A 211 | | 19.577 110.022 | 1.00 45.94 |
| | | | 20.702 108.654 | 1.00 43.16 |
| MOTA | | | 20.751 109.642 | 1.00 43.98 |
| ATOM | 1677 C GLY A 211 | 24.514 2 | 21.450 110.911 | 1.00 45.01 |
| MOTA | 1678 0 GLY A 211 | | 22.479 110.858 | 1.00 48.15 |
| MOTA | 1679 N LYS A 212 | | 20.896 112.059 | 1.00 41.63 |
| MOTA | 1680 CA LYS A 212 | | 21.495 113.328 | |
| ATOM | 1681 CB LYS A 212 | | | 1.00 45.07 |
| | | 23.913 2 | 0.715 114.490 | 1.00 46.59 |
| ATOM | | 22.386 2 | 0.591 114.462 | 1.00 55.31 |
| MOTA | 1683 CD LYS A 212 | 21.651 2 | 1.945 114.481 | 1.00 57.42 |
| MOTA | 1684 CE LYS A 212 . | 21.749 2 | 2.696 113.151 | 1.00 59.71 |
| ATOM | 1685 NZ LYS A 212 | | 4.017 113.178 | 1.00 57.43 |
| MOTA | 1686 C LYS A 212 | | 1.513 113.469 | 1.00 42.08 |
| ATOM | 1687 0 LYS A 212 | | | |
| ATOM | | | 2.326 114.207 | 1.00 40.03 |
| | | | 0.615 112.751 | 1.00 39.51 |
| ATOM | 1689 CA GLY A 213 | | 0.538 112.817 | 1.00 40.11 |
| MOTA | 1690 C GLY A 213 | 28.888 2 | 1.519 111.916 | 1.00 38.25 |
| ATOM | 1691 O GLY A 213 | | 1.575 111.913 | 1.00 34.70 |
| MOTA | 1692 N LYS A 214 | | 2.295 111.143 | 1.00 37.31 |
| ATOM | 1693 CA LYS A 214 | | | |
| ATOM | 1694 CB LYS A 214 | | | 1.00 39.58 |
| | | | 4.017 109.463 | 1.00 44.69 |
| MOTA | 1695 CG LYS A 214 | | 5.030 108.461 | 1.00 44.53 |
| MOTA | 1696 CD LY: A 214 | 27.047 2 | 5.704 107.720 | 1.00 47.71 |
| ATOM | 1697 CE LY. A 214 | 27.553 2 | 6.759 106.754 | 1.00 52.94 |
| MOTA | 1698 NZ LYL A 214 | | 6.183 105.717 | 1.00 57.45 |
| ATOM | 1699 C LYS A 214 | | 4.259 111.085 | |
| ATOM | 1700 O LYS A 214 | | | 1.00 40.16 |
| | | | 4.963 111.933 | 1.00 37.92 |
| ATOM | 1701 N GLY A 215 | | 4.295 110.846 | 1.00 36.57 |
| ATOM | 1702 CA GLY A 215 | 31.716 25 | 5.183 111.593 | 1.00 35.03 |
| ATOM | 1703 C GLY A 215 | | 4.448 112.709 | 1.00 34.57 |
| ATOM | 1704 O GLY A 215 | | 5.039 113.454 | 1.00 33.76 |
| ATOM | 1705 N TYR A 216 | | | |
| | | | 3.153 112.837 | 1.00 34.61 |
| ATOM | 1706 CA TYR A 216 | | 2.378 113.885 | 1.00 35.00 |
| ATOM | 1707 CB TYR A 216 | | 1.683 114.753 | 1.00 36.19 |
| ATCM | 1708 CG TYR A 216 | 30.928 22 | 2.671 115.547 | 1.00 36.68 |
| MOTA | 1709 CD1 TYR A 216 | | .462 114.925 | 1.00 35.83 |
| ATOM | 1710 CE1 TYR A 216 | | .431 115.641 | 1.00 40.89 |
| | 1711 CD2 TYR A 216 | | | |
| ATOM | | | 1.869 116.910 | 1.00 41.50 |
| MOTA | 1712 CE2 TYR A 216 | | .834 117.634 | 1.00 40.69 |
| ATOM | 1713 CZ TYR A 216 | 29.505 24 | .612 116.994 | 1.00 40.17 |
| ATOM | 1714 OH TYR A 216 | 28.816 25 | .566 117.708 | 1.00 38.09 |
| ATOM | 1715 C TYR A 216 | | .384 113.401 | 1.00 34.05 |
| | 1716 O TYR A 216 | | .462 114.127 | 1.00 31.87 |
| MOTA | 7.23 O 11K 11 220 | 24.202 20 | .402 TT# .TE/ | 1.00 31.87 |
| | | | | |

```
1717
  ATOM
                 N
                     ASN A 217
                                     34.343
                                              21.580 112.170
                                                               1.00 29.90
  ATOM
          1718
                 CA
                     ASN A 217
                                     35.398
                                              20.748 111.606
                                                               1.00 30.02
  MOTA
          1719
                 CB
                     ASN A 217
                                     34.833
                                              19.727 110.615
                                                               1.00 26.46
          1720
  MOTA
                 CG
                     ASN
                         A 217
                                     35.897
                                              18.764 110.105
                                                               1.00 30.13
          1721
                     ASN A 217
  ATOM
                 OD1
                                     36.558
                                              19.022 109.097
                                                               1.00 29.80
  ATOM
          1722
                ND2
                     ASN A 217
                                     36.094
                                              17.659 110.831
                                                               1.00 19.92
  MOTA
          1723
                С
                     ASN A 217
                                     36.378
                                              21.686 110.915
                                                               1.00 30.23
          1724
                     ASN A 217
  ATOM
                0
                                     35.983
                                              22.502 110.080
                                                               1.00 27.88
  ATOM
          1725
                N
                     LEU A 218
                                     37.655
                                              21.577 111.271
                                                               1.00 29,45
  ATOM
          1726
                CA
                     LEU A 218
                                     38.670
                                              22.451 110.698
                                                               1.00 28.76
          1727
  ATOM
                CB
                     LEU A 218
                                     39.160
                                              23.444 111.753
                                                               1.00 29.02
                                     39.513
  MOTA
          1728
                CG
                     LEU A 218
                                              24.867
                                                     111.307
                                                               1.00 34.69
          1729
 ATOM
                CD1
                    LEU A 218
                                     40.432
                                              25.480 112.367
                                                               1.00 32.93
          1730
 ATOM
                CD2
                    LEU A 218
                                     40.197
                                             24.873 109.954
                                                               1.00 30.69
 ATOM
          1731
                С
                     LEU A 218
                                     39.870
                                             21.657
                                                     110.207
                                                               1.00 26.65
          1732
                    LEU A 218
 ATOM
                0
                                     40.527
                                             20.981 110.999
                                                               1.00 25.25
          1733
 ATOM
                N
                    ASN A 219
                                     40.151
                                             21.752 108.909
                                                               1.00 25.21
 ATOM
         1734
                CA
                    ASN A 219
                                     41.287
                                             21.069
                                                     108,294
                                                               1.00 21.91
 ATOM
         1735
                CB
                    ASN A 219
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                                             20.314 107.018
                                                               1.00 23.69
         1736
 ATOM
                CG
                    ASN A 219
                                     39.972
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                OD1
                    ASN A 219
                                    40.153
                                             18.440 108.289
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                    ASN A 219
         1738
 MOTA
                ND2
                                    39.018
                                             18.900 106.407
                                                              1.00 24.48
         1739
 ATOM
                C
                    ASN A 219
                                     42.355
                                             22.074 107.906
                                                              1.00 23.46
 ATOM
         1740
                O
                    ASN A 219
                                    42.059
                                             23.073 107.259
                                                              1.00 28.17
 ATOM
         1741
                N
                    ILE A 220
                                    43.595
                                             21.804 108.287
                                                              1.00 23.90
 ATOM
         1742
                CA
                    ILE A 220
                                    44.702
                                             22.684 107.945
                                                              1.00 23.22
 ATOM
         1743
                CB
                   ILE A 220
                                    45.468
                                             23.131 109.212
                                                              1.00 28.73
         1744
 ATOM
                CG2
                   ILE A 220
                                    46.601
                                            24.078 108.831
                                                              1.00 26.01
         1745
 MOTA
                CG1
                   ILE A 220
                                    44.502
                                             23.783 110.212
                                                              1.00 26.36
         1746
 ATOM
                CD1
                    ILE A 220
                                    43.771
                                            25.004 109.688
                                                              1.00 25.74
         1747
 ATOM
               C
                    ILE A 220
                                    45.669
                                            21.929 107.018
                                                              1.00 25.29
         1748
 ATOM
               0
                    ILE A 220
                                    46.631
                                            21.315
                                                    107.477
                                                              1.00 20.44
         1749
 MOTA
               N
                    PRO A 221
                                    45.396
                                            21.924, 105.703
                                                              1.00 26.34
        1750
 ATOM
               CD
                    PRO A 221
                                    44.234
                                            22:497 104.999
                                                              1.00 28.22
 ATOM
        1751
               CA
                    PRO A 221
                                    46.271
                                            21.234 104.747
                                                              1.00 26.92
        1752
 MOTA
               CB
                   PRO A 221
                                    45.454
                                            21.279
                                                    103.457
                                                              1.00 27.81
        1753
 ATOM
               CG
                   PRO A 221
                                    44.774
                                            22.622 103.582
                                                              1.00 30.62
        1754
 ATOM
               C
                   PRO A 221
                                    47.595
                                            21.977
                                                    104.625
                                                              1.00 27.45
        1755
               0
 MOTA
                   PRO A 221
                                   47.603
                                            23.199
                                                    104.457
                                                              1.00 31.21
        1756
 MOTA
               N
                   LEU A 222
                                            21.242 104.703
                                   48.704
                                                              1.00 26.01
 MOTA
        1757
               CA
                   LEU A 222
                                   50.038
                                            21.838 104.640
                                                              1.00 26.41
        1758
 ATOM
               CB
                   LEU A 222
                                   50.726
                                            21.650 105.997
                                                              1.00 26.12
ATOM
        1759
               CG
                   LEU A 222
                                   49.960
                                            22.322
                                                    107.150
                                                              1.00 27.67
        1760
              CD1
ATOM
                   LEU A 222
                                                   108.497
                                   50.531
                                            21.899
                                                              1.00 30.97
        1761
ATOM
              CD2
                   LEU A 222
                                   50.024
                                            23.839 106.985
                                                              1.00 31.59
                   LEU À 222
ATOM
        1762
              C
                                   50.911
                                            21.286 103.504
                                                              1.00 28.97
        1763
MOTA
              O
                   LEU A 222
                                   50.784
                                            20.128 103.117
                                                             1.00 27.95
        1764
                                   51.821
52.059
ATOM
              N
                   PRO A 223
                                            22.116 102.964
                                                             1.00 31.52
ATOM
        1765
              CD
                   PRO A 223
                                            23.518
                                                   103.358
                                                             1.00 29.08
ATOM
        1766
              CA
                   PRO A 223
                                   52.727
                                            21.753 101.865
                                                             1.00 29.93
       1767
ATOM
              CB
                   PRO A 223
                                   53.265
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ATOM
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              CG
                  PRO A 223
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MOTA
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              C
                  PRO A 223
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       1770
ATOM
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                  PRO A 223
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MOTA
       1771
              N
                  LYS A 224
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       1772
MOTA
              CA
                  LYS A 224
                                   55.595
                                           19.320
                                                   101.264
                                                                  32.88
                                                             1.00
       1773
MOTA
              CB
                  LYS
                      A 224
                                  55.938
                                           18.767
                                                    99.884
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       1774
                                  54.761
ATOM
              CG
                  LYS
                      A 224
                                           18.204
                                                    99.115
                                                             1.00 39.37
MOTA
       1775
              CD
                  LYS A 224
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                                                    97.658
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       1776
ATOM
             CE
                  LYS
                      A 224
                                  53.989
                                           17.478
                                                    96.835
                                                             1.00 47.90
       1777
                                  54.331
             NZ
                  LYS
                      A 224
ATOM
                                           17.441
                                                    95.388
                                                             1.00 46.50
       1778
                  LYS A 224
             C
atom
                                  56.817
                                           20.054 101.798
                                                             1.00 29.43
MOTA
       1779
             O
                  LYS
                      A 224
                                  56.933
                                                   101.640
                                           21,270
                                                             1.00 24.10
       1780
                  GLY A 225
             N
                                  57.735
ATOM
                                           19.305
                                                   102.403
                                                             1.00
                                                                  25.00
       1781
                 GLY A 225
             CA
ATCM
                                  58.947
                                           19.896 102.942
                                                             1.00
                                                                  26.20
       1782
             C
                  GLY A 225
ATOM
                                  58.727
                                           20.792 104.154
                                                             1.00 29.44
```

| ATC | OM 1783 O GLY A 225 | 59.610 21.562 104 528 1 00 20 00 |
|---------|----------------------|---|
| ATO | | 50 100 201.020 1.00 29.00 |
| ATO | 1. ZZU | 37.360 20.679 104.777 1.00 24 26 |
| ATO | OM 1786 CB LEU A 226 | 3/.212 21.488 105.951 1.00 25 36 |
| | 320 A 220 | 33.930 20.925 106.579 1.00.23 22 |
| ATC | | 55.172 21.757 107.611 1.00 28.28 |
| ATC | 101 DD0 A 220 | 2.00 20.20 |
| ATO | M 1789 CD2 LEU A 226 | 7 200 40.07 |
| ATO | M 1790 C LEU A 226 | 50 770 |
| ATO | M 1791 O LEU A 226 | 24,79 |
| ATO | M 1792 N ASN A 227 | 58.902 20.450 107.299 1.00 26.15 |
| ATO | 22, | 38.664 22.674 107.548 1.00 23.94 |
| ATO | | 39.702 22.733 108.578 1.00 24 Bo |
| | 11011 11 22 / | 60.751 23.823 108.269 1.00 27.43 |
| ATO | | 60.190 25.231 108.334 1.00 31.62 |
| ATO: | | 50 505 |
| ATO | | 2.00 31.17 |
| ATO | M 1798 C ASN A 227 | 55 55 55 55 55 55 55 55 55 55 55 55 55 |
| ATO | M 1799 O ASN A 227 | |
| ATO | M 1800 N ASP A 228 | 57.873 23.206 110.065 1.00 18.45 |
| ATO | | 59.880 22.862 111.018 1.00 21.29 |
| ATO | 220 | 39.357 23.032 112.375 1.00 25 80 |
| ATON | | 60.464 22.893 113.426 1.00 24 02 |
| | | 61.110 21.520 113.422 1.00 26.48 |
| ATON | | 60.410 20.530 113.135 1.00 29.55 |
| ATOM | | 50 29,35 |
| ATOM | 1 1806 C ASP A 228 | EQ 400 23.00 |
| ATOM | 1 1807 O ASP A 228 | |
| ATOM | 1 1808 N ASN A 229 | E0 455 == 1.00 25.00 |
| ATOM | 1809 CA ASN A 229 | 1.00 43.78 |
| ATOM | | 1.00 27.75 |
| ATOM | | 59.453 27.850 111.770 1.00 32.77 |
| ATOM | | 28.020 112.621 1.00 30.35 |
| ATOM | 1813 ND2 ASN A 229 | 00.035 28.433 113.782 1.00 33.12 |
| ATOM | | 61.856 27.691 112 ₋ 053 1 00 20 11 |
| | | 27.168 26.817 111 645 1 00 20 42 |
| ATOM | | 56.230 27.387 112.202 1.00 26.75 |
| MOTA | | 57.041 26:228 110.463 1.00 30.80 |
| ATOM | | |
| ATOM | 1818 CB GLU A 230 | 55 000 |
| ATOM | 1819 CG GLU A 230 | EC 000 45.11 |
| ATOM | 1820 CD GLU A 230 | 1.00,35.94 |
| MOTA | 1821 CE1 GLU A 230 | |
| MOTA | 1822 OE2 GLU A 230 | EC 057 38.98 |
| ATOM | 1823 C GLU A 230 | |
| MOTA | 1824 O GLU A 230 | 1.00 30.13 |
| ATOM | 1825 N PHE A 231 | 53.563 25.799 110.631 1.00 28.35 |
| ATOM | 1826 CA PHE A 231 | 55.141 24.262 111.060 1.00 32.49 |
| ATOM | | 34.223 23.386 111.790 1.00 28 54 |
| ATOM | | 54.913 22.075 112.191 1.00 31.22 |
| | | 53.974 21.050 112.781 1.00 28 41 |
| ATOM | 1829 CD1 PHE A 231 | 53.026 20.417 111.982 1 00 29 66 |
| ATOM | 1830 CD2 PHE A 231 | 54.036 20.723 114.130 1.00 28.38 |
| ATOM | 1831 CE1 PHE A 231 | 52.153 19.469 112.518 1.00 25.79 |
| ATOM | 1832 CE2 PHE A 231 | |
| ATOM | 1833 CZ PHE A 231 | 1.00 31.40 |
| ATOM | 1834 C PHE A 231 | |
| ATOM | 1835 O PHE A 231 | 1.00 20.05 |
| MOTA | 1836 N LEU A 232 | 2.00 23.33 |
| ATOM | 1837 CA LEU A 232 | 1.00 20./5 |
| ATOM | 1838 CB LEU A 232 | 54.193 25.283 115.092 1.00 27.25 |
| ATOM | | 33.422 25.617 115.933 1.00 25.15 |
| | | 56.1/6 24.372 116.420 1.00 28.11 |
| ATOM | 1840 CD1 LEU A 232 | 57.440. 24.783 117.162 1.00 27.32 |
| ATOM | 1841 CD2 LEU A 232 | 55.268 23.540 117.328 1.00 27.87 |
| ATOM | 1842 C LEU A 232 | 53.371 26.542 114.800 1.00 26 99 |
| ATOM | 1843 O LEU A 232 | 52.449 26.866 115.544 1.00 23.34 |
| ATOM | 1844 N PHE A 233 | 53.694 27.232 113.708 1.00 24.99 |
| ATOM | 1845 CA PHE A 233 | 1,00 24,39 |
| ATCM | 1646 CB PHE A 233 | 1.00 20.13 |
| ATOM | 1847 CG PHE A 233 | |
| ATOM | 1948 CD1 PHE A 233 | |
| | | 52.803 31.441 111.962 1.00 32.80 |
| | | |

| | | | | | • | | | |
|--------------|------|------|-------------|---|------------------|--------|--------------------|--------------------------|
| ATOM | 1849 | CI | 2. PHE A 23 | 3 | 51.825 | 29.903 | 3 110.412 | 1.00 31.59 |
| ATOM | 1850 | | | | 52.008 | | 3 111.452 | |
| ATOM | 1851 | L CE | | | 51.022 | | | |
| ATOM | 1852 | . C2 | | | 51.114 | | 3 110.415 | 1.00 32.50 |
| ATOM | 1853 | | PHE A 23 | | 51.510 | | 113.031 | 1.00 31.62 |
| ATOM | 1854 | | PHE A 23 | | 50.553 | | 113.532 | 1.00 25.88 |
| ATOM | 1855 | | ALA A 23 | | 51.370 | | 112.215 | 1.00 28.12 |
| ATOM | 1856 | | | | 50.056 | | 111.853 | |
| ATOM | 1857 | | | | 50.195 | | 110.864 | 1.00 20.08 |
| ATOM | 1858 | | ALA A 23 | | 49.304 | | 113.089 | 1.00 20.08 |
| ATOM | 1859 | | ALA A 23 | | 48.114 | | 113.089 | 1.00 25.17 |
| MOTA | 1860 | | LEU A 23 | | 50.002 | • - | 113.234 | 1.00 25.21 |
| ATOM | 1861 | | | | 49.367 | | 115.195 | |
| ATOM | 1862 | | | | 50.356 | | 116.026 | 1.00 33.70 1.00 32.70 |
| | 1863 | | | | 49.772 | | 116.020 | |
| ATOM | 1864 | | 1 LEU A 23 | | 50.634 | | 118.052 | 1.00 36.89 |
| MOTA | 1865 | | | | 48.344 | | 117.231 | 1.00 31.37 |
| MOTA | 1866 | | LEU A 23 | | 48.841 | | | 1.00 31.47 |
| MOTA | 1867 | | LEU A 23 | | 47.673 | | 116.062 116.455 | 1.00 33.38 |
| MOTA | 1868 | | GLU A 23 | | | | | 1.00 28.13 |
| ATOM | 1869 | | GLU A 236 | | 49.710 49.336 | | 116.362 | 1.00 34.02 |
| ATOM | 1870 | | GLU A 236 | | | | 117.199 | 1.00 37.30 |
| MOTA | 1871 | CG | GLU A 236 | | 50.528 51.675 | | 117.400 | 1.00 41.51 |
| MOTA | 1872 | CD | GLU A 236 | | | | 118.188 | 1.00 49.54 |
| ATOM | 1873 | OE: | | | 52.811 | | 118.451 | 1.00 55.02 |
| ATOM | 1874 | OE | | | 53.781 | | 119.140 | 1.00 56.19 |
| MOTA | 1875 | C. | GLU A 236 | | 52.735 | | 117.968 | 1.00 54.84 |
| ATOM | 1876 | Ö | GLU A 236 | | 48.163 | | 116.638 | 1.00 33.98 1.00 37.01 |
| ATOM | 1877 | N | LYS A 237 | | 47.211 48.223 | | 117.362 | |
| ATOM | 1878 | CA | LYS A 237 | | 47.140 | | 115.354 114.726 | 1.00 33.94 1.00 33.10 |
| ATOM | 1879 | CB | LYS A 237 | | 47.505 | | 113.281 | |
| ATOM | 1880 | CG | LYS A 237 | | 48.695 | | 113.261 | 1.00 36.08 |
| ATOM | 1881 | CD | LYS A 237 | | 48.395 | | | 1.00 33.62 |
| MOTA | 1882 | CE | LYS A 237 | | 49.569 | | 113.856 113.762 | 1.00 37.99 1.00 45.24 |
| ATOM ATOM | 1883 | NZ | LYS A 237 | | 49.285 | | 114.500 | 1.00 43.24 |
| ATOM | 1884 | C | LYS A 237 | | 45.820 | | 114.751 | 1.00 43.49 |
| ATOM | 1885 | ō | LYS A 237 | | 44.793 | | 115.131 | 1.00 31.40 |
| ATOM | 1886 | N | SER A 238 | | 45.841 | | 114.354 | 1.00 28.72 |
| ATOM | 1887 | CA | SER A 238 | | 44.610 | | 114.335 | 1.00 20.72 |
| ATOM . | 1888 | CB | SER A 238 | | 44.834 | | 113.660 | 1.00 28.90 |
| ATOM | 1889 | OG | SER A 238 | | 45.760 | | 114.372 | 1.00 25.18 |
| ATOM | 1890 | c | SER A 238 | | 44.041 | | 115.740 | 1.00 33.23 |
| ATOM | 1891 | ō | SER A 238 | | 42.823 | | 115.916 | 1.00 34.79 |
| ATOM | 1892 | N | LEU A 239 | | 44.907 | | 116.741 | 1.00 35.27 |
| ATOM | 1893 | CA | LEU A 239 | | 44.413 | | 118.108 | 1.00 37.57 |
| ATOM | 1894 | CB | LEU A 239 | | 45.554 | | 119.090 | 1.00 38.58 |
| ATOM | 1895 | CG | LEU A 239 | | 46.176 | | 119.038 | 1.00 39.74 |
| ATOM | 1896 | | LEU A 239 | | 47.276 | | 120.075 | 1.00 35.82 |
| ATOM | 1897 | | LEU A 239 | | 45.109 | | 119.301 | 1.00 34.93 |
| ATOM | 1898 | c | LEU A 239 | | 43.670 | | 118.521 | 1.00 39.09 |
| ATOM | 1899 | õ | LEU A 239 | | 42.628 | | 119.174 | 1.00 35.50 |
| ATOM | 1900 | N | GLU A 240 | | 44.202 | | 118.131 | 1.00 39.27 |
| ATOM | 1901 | CA | GLU A 240 | | 43.561 | | 118.450 | 1.00 40.15 |
| | 1902 | СВ | GLU A 240 | | 44.366 | | 117.883 | 1.00 40.42 |
| MOTA MOTA | 1903 | CG | GLU A 240 | | 45.661 | | 118.602 | 1.00 43.91 |
| ATOM | 1904 | CD | GLU A 240 | | 46.407 | | 117.942 | 1.00 49.31 |
| ATOM | 1905 | | GLU A 240 | | 45.772 | | 117.665 | 1.00 49.00 |
| ATOM | 1906 | OE2 | | | 47.624 | 32.745 | 117.705 | 1.00 54.05 |
| | 1907 | C | GLU A 240 | | 42.165 | 30.712 | 117.849 | 1.00 39.58 |
| ATOM | 1908 | ō | GLU A 240 | | 41.224 | 30.312 | 118.455 | 1.00 40.99 |
| MOTA | 1909 | N | ILE A 241 | | 42.039 | 20.022 | 116.645 | 1.00 35.70 |
| ATCM | 1909 | CA | ILE A 241 | | 40.754 | 20 774 | 115.964 | 1.00 38.23 |
| ATOM | 1911 | CB | ILE A 241 | | 40.754 | 20 150 | 114.546 | 1.00 37.55 |
| MOTA | 1911 | CG2 | ILE A 241 | | 39.535 | 20 NNE | 113.895 | 1.00 37.30 |
| ATOM | | CG2 | ILE A 241 | | 41.832 | 30 040 | 113.724 | 1.00 37.36 |
| ATOM | 1913 | | ILE A 241 | | 42.106 | 30.048 | 112.320 | 1.00 36.36 |
| ATOM | 1914 | דעני | The w sat | | 45.T00 | 29.541 | 116.36U | T.00 30.T3 |

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| ATOM | 1915 C ILE A 241 | | 39.75 | 1 28.881 116.737 1.00 37.31 |
|--------------|---|---|------------------|--|
| ATOM | | | 38.59 | |
| ATOM | | | 40.20 | 3 27.732 117.231 1.00 37.07 |
| ATOM | | | 39.33 | |
| ATOM | | | 40.02 | 5 25.477 118.250 1.00 37.58 |
| MOTA | | | 39.120 |) 24.581 119.078 1.00 31.91 |
| ATOM | | | 40.364 | 24.803 116.928 1.00 39.21 |
| MOTA | | | 38.930 | |
| MOTA MOTA | | | 37.759 | |
| ATOM | | | 39.905 | |
| ATOM | | • | 39.661 | |
| ATOM | | | 40.945 41.853 | 21.01 |
| ATOM | | | 41.250 | |
| ATOM | 1929 CE LYS A 243 | | 41.054 | |
| ATOM | 1930 NZ LYS A 243 | | 40.448 | |
| ATOM | 1931 C LYS A 243 | | 38.559 | |
| ATOM | 1932 O LYS A 243 | | 37.815 | |
| MOTA | 1933 N GLU A 244 | | 38.451 | |
| MOTA | 1934 CA GLU A 244 | | 37.460 | 31.471 120.004 1.00 54.74 |
| ATOM | 1935 CB GLU A 244 | | 37.954 | 32.497 118.986 1.00 55.15 |
| MOTA | 1936 CG GLU A 244 | | 37.068 | 33.717 118.865 1.00 60.63 |
| ATOM ATOM | 1937 CD GLU A 244 1938 OE1 GLU A 244 | | 37.602 | 34.714 117.868 1.00 65.87 |
| ATOM | 1939 OE2 GLU A 244 | | 38.746 | 35.181 118.053 1.00 70.36 |
| ATOM | 1940 C GLU A 244 | | 36.879 36.051 | 35.031 116.900 1.00 67.09 |
| ATOM | 1941 O GLU A 244 | | 35.127 | 31.025 119.626 1.00 52.65 31.838 119.606 1.00 55.59 |
| ATOM | 1942 N VAL A 245 | | 35.869 | 31.838 119.606 1.00 55.59 29.745 119.332 1.00 50.57 |
| ÁTOM | 1943 CA VAL A 245 | | 34.546 | 29.269 118.947 1.00 45.75 |
| ATOM | 1944 CB VAL A 245 | | 34.475 | 29.081 117.409 1.00 46.91 |
| MOTA | 1945 CG1 VAL A 245 | | 33.085 | 28.634 116.986 1.00 52.62 |
| ATOM | 1946 CG2 VAL A 245 | | 34.825 | 30.389 116.716 1.00 48.34 |
| MOTA | 1947 C VAL A 245 | | 34.130 | 27.969 119.642 1.00 42.67 |
| MOTA | 1948 O VAL A 245 1949 N PHE A 246 | | 33.021 | 27.480 119.445 1.00 43.61 |
| MOTA MOTA | 1949 N PHE A 246 1950 CA PHE A 246 | | 35.001 | 27.417 120.477 1.00 40.87 |
| MOTA | 1951 CB PHE A 246 | | 34.662 35.106 | 26.168 121.139 1.00 37.47 24.991 120.257 1.00 37.00 |
| ATOM | 1952 CG PHE A 246 | | 34.450 | |
| ATOM | 1953 CD1 PHE A 246 | | 33.111 | 23.685 120.604 1.00 33.22 23.467 120.302 1.00 33.93 |
| ATOM | 1954 CD2 PHE A 246 | | 35.168 | 22.674 121.234 1.00 32.13 |
| MOTA | 1955 CE1 PHE A 246 | | 32.493 | 22.260 120.621 1.00 37.75 |
| ATOM | 1956 CE2 PHE A 246 | | 34.561 | 21.459 121.561 1.00 35.92 |
| MOTA | 1957 CZ PHE A 246 | | 33.217 | 21.252 121.251 1.00 36.30 |
| ATOM | 1958 C PHE A 246 1959 O PHE A 246 | | 35.322 | 26.065 122.509 1.00 38.93 |
| MOTA | | | 36.546 | 26.158 122.630 1.00 40.66 |
| ATOM | 1960 N GLU A 247 1961 CA GLU A 247 | | 34.500 34.970 | 25.870 123.537 1.00 38.59 |
| ATOM | 1962 CB GLU A 247 | | 34.146 | .5.733 124.918 1.00 44.60 :5.615 125.865 1.00 47.07 |
| MOTA | 1963 CG GLU A 247 | | 33.161 | 27.569 125.185 1.00 47.07 1.00 1.00 1.00 1.00 1.00 1.00 1.00 |
| ATOM | 1964 CD GLU A 247 | | 31.944 | 26.865 124.577 1.00 62.03 |
| ATOM | 1965 OE1 GLU A 247 | | 32.096 | 26.088 123.607 1.00 61.85 |
| MOTA | 1966 OE2 GLU A 247 | | 30.822 | 27.094 125.083 1.00 64.59 |
| MOTA | 1967 C GLU A 247 | | 34.774 | 24.269 125.285 1.00 39.40 |
| Mota | 1968 O GLU A 247 | | 33.727 | 23.879 125.794 1.00 39.91 |
| MOTA | 1969 N PRO A 248 | | 35.792 | 23.442 125.041 1.00 38.64 |
| ATOM | 1970 CD PRO A 248 | | 37.101 | 23.817 124.483 1.00 33.25 |
| | 1971 CA PRO A 248 1972 CB PRO A 248 | | 35.769 | 22.006 125.316 1.00 35.84 |
| MOTA MOTA | 1972 CB PRO A 248 1973 CG PRO A 248 | | 37.047 37.970 | 21.531 124.648 1.00 36.05 |
| ATOM | 1974 C PRO A 248 | | 35.736 | 22.687 124.982 1.00 34.21 21.611 126.779 1.00 33.94 |
| ATOM | 1975 0 PRO A 248 | | 36.445 | |
| ATOM | 1976 N GLU A 249 | | 34.914 | 22.186 127.597 1.00 32.05 20.616 127.096 1.00 29.39 |
| ATOM | 1977 CA GLU A 249 | | 34.841 | 20.105 128.459 1.00 33.12 |
| ATOM · | 1978 CB GLU A 249 | | 33.521 | 19.361 128.693 1.00 30.36 |
| ATCM | 1979 CG GLU A 249 | | 32.284 | 20.212 128.564 1.00 35.98 |
| atcm | 1980 CD GLU A 249 | | 31.026 | 19.388 128.668 1.00 40.52 |
| | | | | |

| ATOM | 1981 | . OE | 1 GLU Z | 3 249 | | 30.817 | 18.509 | 127.804 | 1.00 40.27 |
|--------|------|------|---------|-------|---|----------------|--------|---------|------------|
| | 1982 | | 2 GLU Z | | | 30.252 | | 129.620 | 1.00 38.57 |
| MOTA | | | | | | | | | |
| MOTA | 1983 | | | A 249 | | 35.995 | | 128.623 | 1.00 32.30 |
| MOTA | 1984 | 0 | GLU Z | A 249 | | 36.472 | 18.884 | 129.728 | 1.00 28.51 |
| MOTA | 1985 | N | VAL 2 | 3 250 | | 36.434 | 18.547 | 127.502 | 1.00 33.74 |
| | 1986 | | | 250 | | 37.516 | | 127.494 | 1.00 29.31 |
| ATOM | | | | | | | | | |
| ATOM | 1987 | | | A 250 | | 36.988 | | 127.926 | 1.00 29.85 |
| MOTA | 1988 | CG: | l VAL A | 1 250 | | 35.908 | 15.711 | 126.958 | 1.00 24.36 |
| ATOM | 1989 | CG: | 2 VAL A | 250 | | 38.121 | 15.166 | 127.978 | 1.00 25.60 |
| - | 1990 | | _VAL 2 | | | 38.066 | | 126.076 | 1.00 29,30 |
| MOTA | | | | | | | | | |
| MOTA | 1991 | 0 | VAL A | | | 37.358 | | 125.114 | 1.00 24.46 |
| ATOM | 1992 | N | TYR A | 251 | | 39.323 | 17.046 | 125.930 | 1.00 27.96 |
| ATOM | 1993 | CA | TYR A | 251 | | 39.865 | 16.913 | 124.585 | 1.00 30.06 |
| | 1994 | СВ | TYR A | | | 40.585 | | 124.165 | 1.00 25.89 |
| MOTA | | | | | | | | | |
| ATOM | 1995 | CG | | 251 | | 41.998 | | 124.692 | 1.00 29.90 |
| MOTA | 1996 | CD. | L TYR A | 251 | | 43.087 | 17.794 | 124.029 | 1.00 26.02 |
| ATOM | 1997 | CE | L TYR A | 251 | | 44.390 | 17.953 | 124.507 | 1.00 29.20 |
| ATOM | 1998 | CD2 | | | | 42.249 | | 125.849 | 1.00 31.96 |
| | | | | | | | | | |
| MOTA | 1999 | CE2 | | | | 43.551 | | 126.338 | 1.00 31.54 |
| ATOM | 2000 | CZ | TYR A | | | 44.614 | 18.694 | 125.664 | 1.00 31.46 |
| MOTA | 2001 | ОН | TYR A | 251 | | 45.894 | 18.854 | 126.152 | 1.00 29.69 |
| ATOM | 2002 | С | TYR A | | | 40.801 | | 124.451 | 1.00 27.56 |
| | | | | | • | | | | |
| ATOM | 2003 | 0 | TYR A | | | 41.382 | | 125.436 | 1.00 28.23 |
| ATOM | 2004 | N | LEU A | | | 40.908 | 15.222 | 123.227 | 1.00 23.52 |
| ATOM | 2005 | CA | LEU A | 252 | | 41.806 | 14.117 | 122.919 | 1.00 26.53 |
| ATOM | 2006 | CB | LEU A | 252 | | 41.057 | 12,930 | 122.293 | 1.00 25.74 |
| | 2007 | CG | LEU A | | | 40.266 | | 123.221 | 1.00 28.49 |
| ATOM | | | | | | | | | |
| MOTA | 2008 | CD1 | | | | 39.122 | | 123.868 | 1.00 27.67 |
| MOTA | 2009 | CD2 | LEU A | 252 | | 39.72 7 | 10.835 | 122.414 | 1.00 32.00 |
| MOTA | 2010 | С | LEU A | 252 | | 42.842 | 14.638 | 121.932 | 1.00 27.53 |
| | 2011 | 0 | LEU A | 252 | • | 42.528 | | 121.055 | 1.00 24.42 |
| ATOM | | | | | | | | | |
| ATOM | 2012 | N | LEU A | | | 44.075 | | 122.078 | 1.00 24.60 |
| MOTA | 2013 | CA | LEU A | | | 45.157 | | 121.204 | 1.00 25.04 |
| ATOM | 2014 | CB | LEU A | 253. | | 46.176 | 15.400 | 122.017 | 1.00 22.48 |
| ATOM | 2015 | CG | LEU A | 253 | | 47.456 | 15.880 | 121.323 | 1.00 21.05 |
| | 2016 | | LEU A | | | 47.105 | | 120.175 | 1.00 23.05 |
| ATOM | | | | | | | | | |
| ATOM | 2017 | | LEU A | | | 48.348 | | 122.360 | 1.00 16.40 |
| ATOM | 2018 | С | LEU A | | | 45.822 | | 120.580 | 1.00 23.55 |
| ATOM | 2019 | 0 | LEU A | 253 | | 46.329 | 12.516 | 121.303 | 1.00 22.11 |
| MOTA | 2020 | N | GLN A | 254 | | 45.811 | 13.287 | 119.248 | 1.00 22.33 |
| | 2021 | CA | GLN A | | | 46.417 | | 118.552 | 1.00 19.84 |
| MOTA | | | | | | | | | |
| MOTA | 2022 | CB | GLN A | | | 45.542 | | 117.348 | 1.00 23.09 |
| ATOM | 2023 | CG | GLN A | 254 | | 46.075 | 12.038 | 115.963 | 1.00 35.49 |
| ATOM | 2024 | CD | GLN A | 254 | | 47.073 | 11.017 | 115.453 | 1.00 31.26 |
| ATOM ' | 2025 | | GLN A | | | 46.712 | | 114.961 | 1.00 33.69 |
| | | | GLN A | | | 48.338 | | 115.574 | 1.00 31.02 |
| : TOM | 2026 | | | | | | | | |
| TOM | 2027 | С | GLN A | | | 47.831 | | 118.153 | 1.00 22.46 |
| FOM | 2028 | 0 | GLN A | 254 | | 48.034 | 13.599 | 117.478 | 1.00 17.56 |
| ATOM | 2029 | N | LEU A | 255 | | 48.804 | 11.781 | 118.590 | 1.00 17.64 |
| | 2030 | CA | LEU A | | | 50.213 | | 118.383 | 1.00 17.04 |
| MOTA | - | | LEU A | | | | | 119.750 | 1.00 14.75 |
| MOTA | 2031 | | | | | | | | |
| ATOM | 2032 | CG | LEU A | | | 50.277 | | 120.670 | 1.00 25.02 |
| ATOM | 2033 | CD1 | LEU A | 255 | | 50.732 | 12.996 | 122.107 | 1.00 21.99 |
| | 2034 | | LEU A | | | 50.636 | | 120.149 | 1.00 18.30 |
| MOTA | | | LEU A | | | 51.023 | 11 160 | 117.476 | 1.00 21.34 |
| ATOM | 2035 | C | | | | | | | |
| ATOM | 2036 | 0 | LEU A | | | 52.089 | | 117.875 | 1.00 18.73 |
| ATOM | 2037 | N | GLY A | 256 | | 50.543 | 10.928 | 116.259 | 1.00 22.75 |
| _ | 2038 | CA | GLY A | 256 | | 51.291 | 10.093 | 115.330 | 1.00 24.09 |
| ATOM | _ | | GLY A | 256 | | 52.660 | 10.721 | 115.126 | 1.00 24.27 |
| MOTA | 2039 | C | | | | | | 115.134 | |
| MOTA | 2040 | 0 | GLY A | | | 52.805 | 11.945 | 113.134 | 1.00 19.15 |
| ATOM | 2041 | N | THR A | | | 53.680 | 9.903 | 114.948 | 1.00 24.14 |
| ATOM | 2042 | CA | THR A | 257 | | 55.014 | 10.440 | 114.765 | 1.00 21.32 |
| | 2043 | CB | THR A | | | 56.048 | 9.582 | 115.511 | 1.00 17.24 |
| MOTA | | | THR A | 257 | | | | 115.004 | 1.00 17.48 |
| ATOM | 2044 | OG1 | TUK A | 257 | | 56.009 | | 117 016 | |
| ATOM: | 2045 | CG2 | THR A | 40/ | | 55.728 | 9.532 | 117.016 | 1.00 15.73 |
| ATOM | 2046 | C | THR A | 257 | | 55.403 | 10.527 | 113.290 | 1.00 22.98 |
| | | | | | | | | | |

| | • | _ | |
|--------------|--|------------------|--|
| ATO | 437 | 56.51 | 7 10.941 112.974 1.00 20.3 |
| ATO | | 54.49 | |
| ATO | | 54.86 | 3 10.229 110.961 1.00 26 5 |
| ATO | 11 230 | 53.849 | 9.496 110.056 1.00 25 0 |
| ATO | | 52.415 | 9.944 110.252 1.00 29 0 |
| IOTA IOTA | 200 | 55.222 | 2 11.596 110.364 1 00 27 8 |
| ATON | | 55.756 |) 11.661 109.254 1.00 25 61 |
| ATON | 1 2055 OD2 ASP A 258 | 52.173 | 11.070 110.742 1.00 29.86 |
| ATOM | | 51.513 | 1.00 33.23 |
| ATOM | | 54.884 54.019 | |
| ATOM | 1 2058 CA PRO A 259 | 55.268 | 1.00 28.55 |
| · ATOM | | 54.447 | ======================================= |
| MOTA | I 2060 CG PRO A 259 | 54.418 | |
| ATOM | | 56.790 | |
| ATOM | | 57.300 | 15.251 110.044 1.00 29.70 |
| MOTA MOTA | | 57.508 | 13.389 111.280 1.00 22.68 |
| ATOM | | 58.960 | 13.545 111.455 1.00 28.41 |
| ATOM | | 59.461 | 12.576 112.533 1.00 22.47 |
| ATOM | 2067 CD1 LEU A 260 | 58.970 | 12.791 113.969 1.00 20.14 |
| ATOM | 2068 CD2 LEU A 260 | 59.352 59.592 | 11.599 114.826 1.00 22.83 |
| ATOM | 2069 C LEU A 260 | 59.770 | 14.079 114.532 1.00 20.48 13.344 110.160 1.00 27.95 |
| MOTA | 2070 O LEU A 260 | 59.407 | |
| ATOM | 2071 N LEU A 261 | 60.874 | 12.535 109.299 1.00 27.03 14.081 110.040 1.00 26.76 |
| ATOM | 2072 CA LEU A 261 | 61.742 | 14.010 108.865 1.00 26 56 |
| ATOM ATOM | 2073 CB LEU A 261 2074 CG LEU A 261 | 63.067 | 14.737 109.137 1.00 23 06 |
| ATOM | 2074 CG LEU A 261 2075 CD1 LEU A 261 | 64.131 | 14.615 108.025 1.00 29 52 |
| ATOM | 2076 CD2 LEU A 261 | 63.642 | 15.325 106.770 1.00 22.68 |
| ATOM | 2077 C LEU A 261 | 65.460 62.063 | 15.219 108.475 1.00 26.71 12.577 108.443 1.00 28.23 |
| MOTA | 2078 O LEU A 261 | 61.880 | |
| ATOM | 2079 N GLU A 262 | 62.539 | 12.198 107.289 1.00 26.52 11.787 109.397 1.00 28.70 |
| ATOM | 2080 CA GLU A 262 | 62.938 | 10.416 109.135 1.00 31.76 |
| ATOM | 2081 CB GLU A 262 | 63.685 | 9.855 110.351 1.00 29 72 |
| ATOM ATOM | 2082 CG GLU A 262 2083 CD GLU A 262 | 64.890 | 10.683 110.803 1.00 31.33 |
| ATOM | 2083 CD GLU A 262 2084 OE1 GLU A 262 | 64.521 | 11.847 111.708 1.00 28.07 |
| ATOM | 2085 OE2 GLU A 262 | 63.324 65.433 | 12.195 111.789 1.00 28.75 |
| ATOM | 2086 C GLU A 262 | 61.847 | 12.424 112.340 1.00 26.08 9.429 108.721 1.00 28.63 |
| MOTA | 2087 O GLU A 262 | 62.158 | 9.429 108.721 1.00 28.63 8.305 108.350 1.00 29.72 |
| ATOM | 2088 N ASP A 263 | 60.582 | 9.825 108.785 1.00 28.07 |
| MOTA | 2089 CA ASP A 263 | 59.513 | 8.902 108.412 1.00 26.85 |
| ATOM ATOM | 2090 CB ASP A 263 2091 CG ASP A 263 | 58.305 | 9.099 109.333 1.00 25.26 |
| ATOM | 2091 CG ASP A 263 2092 OD1 ASP A 263 | 57.261 | 7.998 109.185 1.00 33.14 |
| ATOM | 2093 OD2 ASP A 263 | 56.638 57.042 | 7.636 110.202 1.00 29.91 |
| ATOM | 2094 C ASP A 263 | 59.150 | 7.509 108.051 1.00 26.56 9.146 106.95 1.00 29.44 |
| ATOM | 2095 O ASP A 263 | | |
| ATOM | 2096 N TYR A 264 | 59.303 | 8.111 106.130 1.00 24.70 8.111 106.130 1.00 27.51 |
| ATOM | 2097 CA TYR A 264 | 59.031 | 8.219 104.696 1.00 33.89 |
| ATOM | 2098 CB TYR A 264 | 59.576 | 7.008 103.935 .1.00 40.44 |
| ATOM ATOM | 2099 CG TYR A 264 | 61.059 | 6.771 104.092 1.00 50.64 |
| ATOM | 2100 CD1 TYR A 264 2101 CE1 TYR A 264 | 61.565 | 6.087 105.199 1.00 54.67 |
| ATOM | 2102 CD2 TYR A 264 | 62.933 | 5.876 105.351 1.00 55.28 |
| ATOM | 2103 CE2 TYR A 264 | 61.960 63.329 | 7.242 103.140 1.00 53.79 |
| ATOM | 2104 CZ TYR A 264 | 63.809 | 7.038 103.282 1.00 56.61 6.354 104.388 1.00 56.22 |
| MOTA | 2105 OH TYR A 264 | 65.161 | 6.354 104.388 1.00 56.22 6.147 104.524 1.00 55.90 |
| MOTA | 2106 C TYR A 264 | 57.581 | 8.394 104.294 1.00 31.33 |
| ATOM | 2107 O TYR A 264 | 57.311 | 8.825 103.178 1.00 27.15 |
| MOTA | 2108 N LEU A 265 | 56.641 | 8.059 105.172 1.00 26.88 |
| MOTA MOTA | 2109 CA LEU A 265 2110 CB LEU A 265 | 55.244 | 8.209 104.792 1.00 24.39 |
| MOTA | 2110 CB LEU A 265 2111 CG LEU A 265 | 54.360 54.663 | 7.189 105.527 1.00 26.55 |
| MOTA | 2112 CD1 LEU A 265 | 54.663 53.464 | 5.724 105.168 1.00 29.80 |
| | CD- 220 A 200 | プラ・ゴロボ | 4.836 105.503 1.00 21.17 |

| ATOM | 2113 | CD2 LEU A 265 | 54.931 | 5.620 103.682 | 1.00 33.35 |
|--------------|--------------|---------------------------------|------------------|----------------------------------|--------------------------|
| ATOM | 2114 | C LEU A 265 | 54.669 | | 1.00 20.81 |
| ATOM | 2115 | | 53.457 | | 1.00 21.30 |
| ATOM | 2116 | | 55.540 | 10.622 104.959 | 1.00 23.23 |
| ATOM | 2117 | | 55.084 | | 1.00 26.30 |
| MOTA | 2118 | | 54.856 | | 1.00 25.16 |
| ATOM | 2119 | | 56.074 | | 1.00 22.92 |
| ATOM | 2120 | | 56.147 | | 1.00 30.17 |
| MOTA | 2121 2122 | | 57.334 | 12.555 104.385 | 1.00 31.65 |
| ATOM ATOM | 2122 | | 55.731 | 13.985 103.757 | 1.00 31.56 |
| ATOM | 2124 | CB LYS A 267 | 56.696 56.140 | 14.873 103.140 15.425 101.834 | 1.00 27.65 |
| ATOM | 2125 | | 55.815 | 14.327 100.819 | 1.00 30.54 1.00 34.13 |
| ATOM | 2126 | | 57.039 | | 1.00 29.09 |
| MOTA | 2127 | CE LYS A 267 | 56.745 | 12.376 99.524 | 1.00 37.61 |
| ATOM | 2128 | NZ LYS A 267 | 57.956 | 11.541 99.272 | 1.00 31.91 |
| MOTA | 2129 | C LYS A 267 | 57.050 | 16.004 104.107 | 1.00 30.85 |
| MOTA | 2130 | O LYS A 267 | 57.624 | 17.017 103.707 | 1.00 27.86 |
| MOTA | 2131 | N PHE A 268 | 56.688 | 15.826 105.377 | 1.00 24.19 |
| MOTA | 2132 | CA PHE A 268 | 57.009 | 16.808 106.412 | 1.00 25.34 |
| MOTA | 2133 | CB PHE A 268 | 56.014 | 16.730 107.579 | 1.00 24.54 |
| MOTA | 2134 2135 | CG PHE A 268 CD1 PHE A 268 | 54.636 | 17.256 107.257 | 1.00 21.68 |
| ATOM ATOM | 2136 | CD2 PHE A 268 | 53.631 54.346 | 17.221 108.216 17.806 106.011 | 1.00 28.65 |
| ATOM | 2137 | CE1 PHE A 268 | 52.357 | 17.728 107.944 | 1.00 25.14 1.00 25.34 |
| ATOM | 2138 | CE2 PHE A 268 | 53.077 | 18.315 105.730 | 1.00 23.79 |
| ATOM | 2139 | CZ PHE A 268 | 52.082 | 18.275 106.702 | 1.00 28.13 |
| MOTA | 2140 | C PHE A 268 | 58.410 | 16.470 106.908 | 1.00 25.66 |
| MOTA | 2141 | O PHE A 2.68 | 58.778 | 15.299 106.994 | 1.00 28.44 |
| MOTA | 2142 | N ASN A 269 | 59.194 | 17.490 107.230 | 1.00 25.81 |
| ATOM | 2143 | CA ASN A 269 | 60.555 | 17.270 107.709 | 1.00 30.60 |
| ATOM | 2144 | CB ASN A 269 | 61.566 | 17.938 106.767 | 1.00 31.97 |
| ATOM ATOM | 2145 2146 | CG ASN A 269 - OD1 ASN A 269 | 61.392 | 17.513 105.317 | 1.00 35.83 |
| ATOM | 2147 | ND2 ASN A 269 | 61.235 61.446 | 16.332 105.020 18.477 104.405 | 1.00 33.93 |
| ATOM | 2148 | C ASN A 269 | 60.723 | 17.843 109.110 | 1.00 33.95 1.00 31.80 |
| ATOM | 2149 | O ASN A 269 | 61.609 | 18.665 109.348 | 1.00 28.13 |
| ATOM | 2150 | N LEU A 270 | 59.888 | 17.397 110.043 | 1.00 29.70 |
| MOTA | 2151 | CA LEU A 270 | 59.954 | 17.918 111.406 | 1.00 26.87 |
| MOTA | 2152 | CB LEU A 270 | 58.575 | 17.833 112.074 | 1.00 26.60 |
| ATOM | 2153 | CG LEU A 270 | 57.392 | 18.425 111.297 | 1.00 29.62 |
| ATOM | 2154 2155 | CD1 LEU A 270 CD2 LEU A 270 | 56.177 | 18.494 112.222 | 1.00 28.54 |
| ATOM ATOM | 2156 | C LEU A 270 | 57.740 60.979 | 19.825 110.790 17.242 112.301 | 1.00 29.40 |
| ATOM | 2157 | O LEU A 270 | 61.490 | 17.242 112.301 16.158 111.990 | 1.00 26.83 1.00 19.60 |
| ATOM | 2158 | N SER A 271 | 61.275 | 17.896 113.420 | 1.00 13.60 |
| ATOM | 2159 | CA SER A 271 | 62.220 | 17.365 114.393 | 1.00 27.08 |
| ATOM | 2160 | CB SER A 271 | 63.189 | 18.460 114.846 | 1.00 24.64 |
| ATOM | 2161 | OG SER A 271 | 62.499 | 19.433 115.626 | 1.00 18.60 |
| MOTA | 2162 | C SER A 271 | 61.454 | 16.868 115.618 | 1.00 23.70 |
| ATOM | 2163 | O SER A 271 | 60.272 | 17.150 115.772 | 1.00 22.56 |
| MOTA | 2164 | N ASN A 272 | 62.157 | 16.129 116.470 | 1.00 28.35 |
| MOTA | 2165 2166 | CA ASN A 272 CB ASN A 272 | 61.649 | 15.593 117.739 | 1.00 31.03 |
| ATOM ATOM | 2167 | CG ASN A 272 | 62.774 62.854 | 14.880 118.498 | 1.00 28.80 |
| MOTA | 2168 | OD1 ASN A 272 | 63.712 | 13.428 118.180 12.709 118.705 | 1.00 36.65 1.00 29.89 |
| ATOM | 2169 | ND2 ASN A 272 | 61.953 | 12.969 117.319 | 1.00 40.80 |
| ATOM | 2170 | C ASN A 272 | 61.167 | 16.695 118.661 | 1.00 31.83 |
| ATOM | 2171 | O ASN A.272 | 60.090 | 16.618 119.261 | 1.00 27.50 |
| ATOM | 2172 | N VAL A 273 | 62.032 | 17.693 118.804 | 1.00 31.49 |
| ATOM | 2173 | CA VAL A 273 | 61.802 | 18.837 119.667 | 1.00 31.58 |
| ATOM | 2174 | CB VAL A 273 | 63.069 | 19.709 119.725 | 1.00 35.80 |
| ATOM | 2175 | CG1 VAL A 273 | 62.804 | 20.988 120.500 | 1.00 48.07 |
| ATOM | 2176 | CG2 VAL A 273 | 64.198 | 18.914 120.381 | 1.00 42.81 |
| ATCM | 2177 2178 | C VAL A 273 O VAL A 273 | 60.608 59.872 | 19.665 119.234 | 1.00 30.13 |
| ATOM | _1/0 | O ATTITUTE OF 17 | 33.014 . | 20.174 120.072 | 1.00 31.44 |

| | | • |
|--------|---|---|
| ATC | 111111111111111111111111111111111111111 | 60.405 19.800 117.929 1.00 24 15 |
| ATO | M 2180 CA ALA A 274 | |
| ATO | M 2181 CB ALA A 274 | 50 747 20 707 117 |
| ATO | M 2182 C ALA A 274 | 59.341 20.780 115.965 1.00 21.85 |
| ATO | | 38.005 19.759 117.789 1.00 25 69 |
| ATO: | A 2/4 | 56.961 20.324 118.132 1.00 23 76 |
| ATO | | 58.122 18.438 117 680 1 00 35 30 |
| | Land R 2/J | 57.015 17.538 117 974 1 00 25 00 |
| ATO | INL A 2/3 | E7 440 |
| ATO | | 56 346 |
| ATO | | En and 11 11 11 11 11 11 11 11 11 11 11 11 11 |
| ATOI | M 2189 CD2 PHE A 275 | 1.00 32.80 |
| ATO | M 2190 CE1 PHE A 275 | E4 040 = 1.00 20,93 |
| OTA | M 2191 CE2 PHE A 275 | FF 3.5 1322 2.00 33.73 |
| ATON | M 2192 CZ PHE A 275 | E4 000 10 10 10 10 10 10 10 10 10 10 10 10 |
| ATON | 4 2193 C PHE A 275 | EC 500 1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1 |
| ATOM | | 56.607 17.712 119.445 1.00 24.63 |
| ATOM | | 33.428 17.877 119.767 1.00 22 40 |
| ATOM | 550 A 2/0 | 57.594 17.673 120.331 1.00 25 45 |
| ATOM | 220 A 2/0 | 57.357 17.837 121.766 1.00 27 94 |
| | 02 DDO A 270 | 58.667 17.692 122 534 1 00 26 12 |
| ATOM | | 58.651 18.132 124 001 1 00 31 15 |
| ATOM | | rn 400 1.00 J1.13 |
| ATOM | 120 11 2 70 | 60 033 17 027 104 53 |
| ATOM | 2201 C LEU A 276 | 56 500 1.00 27.30 |
| ATOM | 2202 O LEU A 276 | TE 000 1 |
| ATOM | 2203 N LYS A 277 | 57 75 222.030 1.00 28.69 |
| ATOM | 2204 CA LYS A 277 | 55 045 100 30.33 |
| ATOM | 2205 CB LYS A 277 | Ch |
| ATOM | 2206 CG LYS A 277 | 37.742 22.516 120.704 1.00 30.38 |
| MOTA | 2207 CD LYS A 277 | 37.941 23.934 121.237 1.00 36.46 |
| MOTA | 2208 CE LYS A 277 | 36.633 24.668 121.454 1.00 42 73 |
| ATOM | 2209 NZ LYS A 277 | 36.870 26.059 122.049 1.00 45 70 |
| ATOM | 210 R 2// | 57.528 26.004 123.390 1.00 44 64 |
| ATOM | | 55.432 21.683 121.242 1.00 30 26 |
| ATOM | n L// | 54.640 22.284 121.972 1.00 27 55 |
| | | 55.057 21.078 120.115 1 00 20 15 |
| ATOM | 2213 CA ALA A 278 | 53.662 21.096 119.676 1.00 30.51 |
| ATOM | 2214 CB ALA A 278 | E3 400 30.31 |
| ATOM | 2215 C ALA A 278 | E2 700 20.90 |
| MOTA | 2216 O ALA A 278 | |
| MOTA | 2217 N PHE A 279 | E3 24E 10 10 10 10 10 10 10 10 10 10 10 10 10 |
| ATOM | . 2218 CA PHE A 279 | |
| MOTA | 2219 CB PHE A 279 | 53 2.62 |
| ATOM | 2220 CG PHE A 279 | 50 20 20.03 |
| ATOM | 2221 CD1 PHE A 279 | C. 2.1 |
| MOTA | 2222 CD2 PHE A 279 | 53 50- |
| MOTA | 2223 CE1 PHE A 279 | 53.505 16.786 125.267 1.00 33.03 |
| ATOM | 2224 CE2 PHE A 279 | 51.054 15.500 125.121 1.00 37.90 |
| ATOM | 2225 CZ PHE A 279 | 53.011 16.114 126.386 1.00 38.01 |
| ATOM | 2226 C PHE A 279 | 51.783 15.469 126.313 1.00 36 17 |
| ATOM | | 52.362 19.730 123.621 1.00 30 67 |
| ATOM | | 51.265 19.853 124.184 1.00 26.26 |
| MOTA | | 53.432 20.429 123.990 1 00 32 03 |
| MOTA | 11 200 | 53.339 21.373 125.104 1.00 30.54 |
| | 2230 CB ASN A 280 | 54.724 21.819 125.583 1.00 26.79 |
| MOTA | 2231 CG ASN A 280 | 55.508 20.695 126.227 1.00 33.68 |
| MOTA | 2232 OD1 ASN A 280 | |
| ATOM | 2233 ND2 ASN A 280 | EC 000 |
| ATOM | 2234 C ASN A 280 | FO 400 |
| MOTA | 2235 O ASN A 280 | 5. 20. 124.701 1.00.30.46 |
| MOTA | 2236 N ILE A 281 | 52 422 |
| MOTA | 2237 CA ILE A 281 | E1 C20 == 1.00 27.32 |
| MOTA | 2238 CB ILE A 281 | E1 070 |
| ATOM | 2239 CG2 ILE A 281 | 31.878 24.517 121.666 1.00 35.08 |
| ATOM . | 2240 CG1 ILE A 281 | 30.776 25.445 121.174 1.00 34 33 |
| ATCM | | 53.253 25.185 121.562 1.00 33.53 |
| | | 53.590 25.694 120.178 1.00 34 88 |
| | 2242 C ILE A 281 | 50.141 23.798 123.329 1 00 31 22 |
| MOTA | 2243 O ILE A 281 | 49.391 24.621 123.854 1.00 30.15 |
| TOM | 2244 N VAL A 282 | 49.723 22.606 122.923 1.00 30.91 |
| | | |

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Figure 18-35

| ATOM 2246 CB YAL A 282 | | | | | | - | | | | |
|--|--------|------|-----|------------|-----|--------|---------|---------|------|-------|
| ATOM 2246 CB JAL A 282 | ATOM | 2245 | CA | VAL A 2 | 32 | 48.332 | 22.214 | 123.081 | 1.00 | 30.76 |
| ATOM 2248 CG2 VAL A 282 46.641 20.158 122.841 1.00 28.66 ATOM 2249 C VAL A 282 47.952 22.236 124.558 1.00 31.39 ATOM 2250 O VAL A 282 46.884 22.715 124.917 1.00 32.70 ATOM 2251 N ARG A 283 48.837 21.720 125.406 1.00 29.86 ATOM 2252 CA ARG A 283 48.837 21.675 126.840 1.00 34.82 ATOM 2253 CB ARG A 283 49.652 20.785 127.519 1.00 31.44 ATOM 2255 CD ARG A 283 49.652 20.785 127.5519 1.00 31.49 ATOM 2255 CD ARG A 283 49.652 19.334 127.661 1.00 29.49 ATOM 2255 CD ARG A 283 50.729 18.539 127.554 1.00 30.78 ATOM 2255 CD ARG A 283 50.730 18.314 128.990 1.00 30.78 ATOM 2255 NEARGA 283 50.730 18.314 128.990 1.00 30.78 ATOM 2255 NEARGA 283 50.730 18.314 128.990 1.00 30.78 ATOM 2255 NEARGA 283 50.730 18.314 128.990 1.00 30.78 ATOM 2258 NH1 ARG A 283 51.826 18.351 129.742 1.00 35.27 ATOM 2260 C ARG A 283 47.830 23.302 128.439 1.00 36.66 ATOM 2261 O ARG A 283 47.830 23.302 128.439 1.00 35.06 ATOM 2261 O ARG A 283 47.830 23.302 128.439 1.00 35.70 ATOM 2262 N GLU A 284 49.350 23.985 126.928 1.00 35.70 ATOM 2266 CD GLU A 284 49.350 23.985 126.928 1.00 35.70 ATOM 2266 CD GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2266 CD GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 48.57 ATOM 2270 O GLU A 284 50.499 26.166 126.799 1.00 48.57 ATOM 2271 O VAL A 285 44.943 20.266 126.799 1.00 48.57 ATOM 2272 CC AVAL A 285 46.039 26.291 127.148 1.00 39.48 ATOM 2278 O GLU A 284 48.309 26.041 127.148 1.00 39.48 ATOM 2278 O GLU A 284 48.309 26.041 127.148 1.00 39.48 ATOM 2278 O GLU A 284 48.309 26.041 127.148 1.00 39.58 ATOM 2279 C GLU A 288 48.4049 127.408 122.408 120.00 37.00 ATOM 2278 O VAL A 285 44.604 127. | MOTA | 2246 | CB | YAL A 2 | 32 | 48.075 | | | | |
| ATOM 2249 CC VAL A 282 | | | | | | | | | | |
| ATOM 2249 C VAL A 282 46.88 22.715 22.36 124.558 1.00 31.39 ATOM 2251 N ARG A 283 48.837 21.720 125.406 1.00 22.86 ATOM 2252 CA ARG A 283 48.837 21.720 125.406 1.00 22.86 ATOM 2253 CE ARG A 283 49.551 12.306 126.840 1.00 31.44 ATOM 2254 CG. ARG A 283 49.551 12.3126.840 1.00 31.44 ATOM 2255 CD ARG A 283 49.551 12.327.554 1.00 31.47 ATOM 2255 CD ARG A 283 50.729 18.539 127.554 1.00 30.78 ATOM 2257 CZ ARG A 283 50.730 18.314 128.990 1.00 30.78 ATOM 2257 CZ ARG A 283 50.730 18.314 128.990 1.00 30.78 ATOM 2258 NH1 ARG A 283 50.730 18.314 128.990 1.00 30.78 ATOM 2259 NH2 ARG A 283 50.730 18.314 129.742 1.00 35.27 ATOM 2250 NZ ARG A 283 50.730 18.314 129.742 1.00 35.27 ATOM 2260 C ARG A 283 47.830 23.302 128.439 1.00 35.06 ATOM 2261 O ARG A 283 47.830 23.302 128.439 1.00 35.06 ATOM 2261 O ARG A 283 47.830 23.302 128.439 1.00 35.70 ATOM 2262 N GLU A 284 49.350 23.985 126.928 1.00 35.70 ATOM 2265 CG GLU A 284 49.350 23.985 126.928 1.00 35.70 ATOM 2266 CD GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2266 CD GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2266 CD GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2267 OEI GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 48.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 48.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 48.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 48.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 48.17 ATOM 2268 OE2 GLU A 284 50.499 26.166 126.799 1.00 48.57 ATOM 2270 O GLU A 284 48.039 26.014 127.148 1.00 39.58 ATOM 2271 O ALL A 285 44.654 26.891 123.693 1.00 36.43 ATOM 2272 CA VAL A 285 44.694 25.588 125.690 1.00 35.58 ATOM 2273 CB VAL A 285 44.694 25.588 125.690 1.00 35.82 ATOM 2275 CC VAL A 285 44.694 25.268 125.691 1.00 35.82 ATOM 2278 O FIRE A 286 43.199 22.722 125.657 1.00 31.05 ATOM 2280 CB PHE A 286 43.1 | | | | | | | | | | |
| ATOM 2251 N ARG A 283 | | | | | | | | | | • |
| ATOM 2251 N ARG A 283 | | | | | | | | | | |
| ATOM 2252 CA ARG A 283 | | | | | | | | | | |
| ATOM 2253 CB ARG A 283 | | | | | | | | | | • |
| ATOM 2255 CG ARG A 283 | MOTA | 2252 | CA | ARG A 28 | 33 | | | | 1.00 | 34.82 |
| ATOM 2256 NB ARG A 283 50.729 18.539 127.554 1.00 30.78 ATOM 2257 CZ ARG A 283 51.826 18.351 129.742 1.00 35.27 ATOM 2258 NH1 ARG A 283 51.826 18.351 129.198 1.00 36.46 ATOM 2259 NH2 ARG A 283 51.742 18.101 131.035 1.00 36.46 ATOM 2261 O ARG A 283 48.561 23.065 127.473 1.00 35.90 ATOM 2261 O ARG A 283 48.561 23.065 127.473 1.00 35.04 ATOM 2262 N GLU A 284 49.350 23.965 126.928 1.00 35.04 ATOM 2263 C G GLU A 284 49.350 23.965 126.928 1.00 35.04 ATOM 2263 C G GLU A 284 49.376 25.348 127.448 1.00 44.17 ATOM 2265 C G GLU A 284 51.917 25.702 127.141 1.00 66.69 ATOM 2266 CD GLU A 284 51.917 25.702 127.141 1.00 66.69 ATOM 2266 CD GLU A 284 53.012 27.738 126.542 1.00 66.69 ATOM 2267 C GLU A 284 53.012 27.738 126.542 1.00 66.69 ATOM 2267 C GLU A 284 48.039 26.014 127.148 1.00 39.24 ATOM 2268 CD2 GLU A 284 48.039 26.014 127.148 1.00 39.24 ATOM 2270 O GLU A 284 48.039 26.014 127.148 1.00 39.24 ATOM 2271 N VAL A 285 46.039 26.294 125.595 1.00 33.75 ATOM 2271 N VAL A 285 46.039 26.294 125.595 1.00 33.75 ATOM 2272 C A VAL A 285 46.039 26.294 125.595 1.00 33.75 ATOM 2273 C C VAL A 285 44.664 26.811 123.693 1.00 33.64 ATOM 2277 C VAL A 285 44.664 26.811 123.693 1.00 37.26 ATOM 2277 C VAL A 285 44.664 26.811 123.693 1.00 37.56 ATOM 2277 C VAL A 285 44.964 25.638 126.192 1.00 38.56 ATOM 2278 N PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2278 C PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2280 CB PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2280 CB PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2280 CB PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2281 CB PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2281 CB PHE A 286 43.159 22.723 125.657 1.00 32.56 ATOM 2282 CD PHE A 286 43.159 22.723 128.015 1.00 33.06 ATOM 2282 CD PHE A 286 41.388 49.91 123.256 1.00 33.06 ATOM 2287 C PHE A 286 41.389 24.257 24.170 122.202 1.00 32.96 ATOM 2287 C C PHE A 286 41.389 24.257 24.170 122.202 1.00 32.96 ATOM 2299 C C GLU A 288 46.910 17.864 132.411 1.00 45.65 ATOM 2290 C C GLU A 2 | _ ATOM | 2253 | CB | ARG A 28 | 33 | | | | 1.00 | 31.44 |
| ATOM 2257 CZ ARG A 283 50.730 18.314 128.990 1.00 30.78 ATOM 2258 NH1 ARG A 283 51.025 18.611 129.198 1.00 35.27 ATOM 2258 NH2 ARG A 283 51.742 18.100 131.035 1.00 35.90 ATOM 2261 C ARG A 283 48.561 23.065 127.473 1.00 35.90 ATOM 2261 C ARG A 283 47.830 23.302 128.439 1.00 35.06 ATOM 2262 N GLU A 284 49.350 23.965 126.928 1.00 35.70 ATOM 2263 CA GLU A 284 49.350 23.302 128.439 1.00 35.70 ATOM 2264 CB GLU A 284 50.995 23.302 128.439 1.00 35.70 ATOM 2265 CG GLU A 284 50.999 26.166 126.799 1.00 44.17 ATOM 2266 CD GLU A 284 50.999 26.166 126.799 1.00 44.17 ATOM 2266 CD GLU A 284 50.999 26.166 126.799 1.00 60.69 ATOM 2267 CELU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2268 CELU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2268 CELU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2267 CELU A 284 47.525 26.783 127.954 1.00 33.75 ATOM 2270 C GLU A 284 47.525 26.783 127.954 1.00 33.75 ATOM 2271 N VAL A 285 47.72 25.704 125.9986 1.00 33.75 ATOM 2271 N VAL A 285 46.205 26.294 125.5992 1.00 33.75 ATOM 2273 CB VAL A 285 46.205 26.294 125.5992 1.00 33.75 ATOM 2275 CG VAL A 285 44.654 26.811 123.693 1.00 34.14 ATOM 2275 CG VAL A 285 44.654 26.811 123.693 1.00 34.14 ATOM 2275 CG VAL A 285 44.964 25.638 126.192 1.00 38.56 ATOM 2277 CA PALE A 285 44.964 25.638 126.192 1.00 38.56 ATOM 2277 CA PALE A 285 44.964 25.638 126.192 1.00 37.56 ATOM 2277 CA PALE A 286 44.964 25.638 126.192 1.00 37.56 ATOM 2278 CB PHE A 286 43.159 22.773 125.657 1.00 37.56 ATOM 2280 CB PHE A 286 43.159 22.773 125.657 1.00 37.56 ATOM 2280 CB PHE A 286 43.159 22.773 125.657 1.00 37.56 ATOM 2280 CB PHE A 286 43.159 22.773 125.657 1.00 37.56 ATOM 2280 CD PHE A 286 43.159 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.159 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.159 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.922 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.922 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.922 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.929 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 41.40 1.7455 1 | ATOM | 2254 | CG. | - ARG A 28 | 3 | 49.551 | 19.334 | 127.061 | 1.00 | 29.49 |
| ATOM 2257 CZ ARG A 283 50.730 18.314 128.990 1.00 30.78 ATOM 2258 NH1 ARG A 283 51.025 18.611 129.198 1.00 35.27 ATOM 2258 NH2 ARG A 283 51.742 18.100 131.035 1.00 35.90 ATOM 2261 C ARG A 283 48.561 23.065 127.473 1.00 35.90 ATOM 2261 C ARG A 283 47.830 23.302 128.439 1.00 35.06 ATOM 2262 N GLU A 284 49.350 23.965 126.928 1.00 35.70 ATOM 2263 CA GLU A 284 49.350 23.302 128.439 1.00 35.70 ATOM 2264 CB GLU A 284 50.995 23.302 128.439 1.00 35.70 ATOM 2265 CG GLU A 284 50.999 26.166 126.799 1.00 44.17 ATOM 2266 CD GLU A 284 50.999 26.166 126.799 1.00 44.17 ATOM 2266 CD GLU A 284 50.999 26.166 126.799 1.00 60.69 ATOM 2267 CELU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2268 CELU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2268 CELU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2267 CELU A 284 47.525 26.783 127.954 1.00 33.75 ATOM 2270 C GLU A 284 47.525 26.783 127.954 1.00 33.75 ATOM 2271 N VAL A 285 47.72 25.704 125.9986 1.00 33.75 ATOM 2271 N VAL A 285 46.205 26.294 125.5992 1.00 33.75 ATOM 2273 CB VAL A 285 46.205 26.294 125.5992 1.00 33.75 ATOM 2275 CG VAL A 285 44.654 26.811 123.693 1.00 34.14 ATOM 2275 CG VAL A 285 44.654 26.811 123.693 1.00 34.14 ATOM 2275 CG VAL A 285 44.964 25.638 126.192 1.00 38.56 ATOM 2277 CA PALE A 285 44.964 25.638 126.192 1.00 38.56 ATOM 2277 CA PALE A 285 44.964 25.638 126.192 1.00 37.56 ATOM 2277 CA PALE A 286 44.964 25.638 126.192 1.00 37.56 ATOM 2278 CB PHE A 286 43.159 22.773 125.657 1.00 37.56 ATOM 2280 CB PHE A 286 43.159 22.773 125.657 1.00 37.56 ATOM 2280 CB PHE A 286 43.159 22.773 125.657 1.00 37.56 ATOM 2280 CB PHE A 286 43.159 22.773 125.657 1.00 37.56 ATOM 2280 CD PHE A 286 43.159 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.159 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.159 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.922 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.922 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.922 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 43.929 22.773 125.657 1.00 30.30 ATOM 2280 CD PHE A 286 41.40 1.7455 1 | ATOM | 2255 | CD | ARG A 28 | 3 | 50.729 | | | 1.00 | 30:67 |
| ATOM 2258 NH1 ARG A 283 51.826 18.351 129.742 1.00 35.27 ATOM 2258 NH1 ARG A 283 51.742 18.100 131.035 1.00 35.90 ATOM 2261 0 ARG A 283 48.561 23.065 127.473 1.00 35.90 ATOM 2261 0 ARG A 283 48.561 23.065 127.473 1.00 35.04 ATOM 2262 N GLU A 284 49.350 23.985 126.928 1.00 35.04 ATOM 2263 C G GLU A 284 49.376 25.348 127.448 1.00 40.93 ATOM 2266 C G GLU A 284 49.376 25.348 127.448 1.00 40.93 ATOM 2265 C G GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2265 C G GLU A 284 51.917 25.702 127.141 1.00 66.69 ATOM 2266 CD GLU A 284 53.012 27.738 126.542 1.00 66.69 ATOM 2267 C GLU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2268 CE2 GLU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2269 C GLU A 284 48.039 26.014 127.148 1.00 39.24 ATOM 2269 C GLU A 284 48.039 26.014 127.148 1.00 39.24 ATOM 2271 N VAL A 285 47.472 25.704 125.986 1.00 63.15 ATOM 2271 C G VAL A 285 46.039 26.291 124.062 1.00 33.75 ATOM 2272 C A VAL A 285 46.039 26.291 124.062 1.00 33.75 ATOM 2277 C C VAL A 285 46.039 26.291 124.062 1.00 33.75 ATOM 2277 C C VAL A 285 44.964 25.638 126.192 1.00 33.75 ATOM 2277 C WAL A 285 44.964 25.638 126.192 1.00 34.14 ATOM 2278 N PHE A 286 44.964 25.638 126.192 1.00 37.26 ATOM 2277 C VAL A 285 44.964 25.638 126.192 1.00 37.26 ATOM 2277 C VAL A 285 44.964 25.638 126.192 1.00 37.26 ATOM 2279 C PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2280 C B PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2280 C B PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2281 C C PHE A 286 43.159 22.723 125.657 1.00 32.55 ATOM 2281 C C PHE A 286 43.159 22.723 125.657 1.00 32.55 ATOM 2282 CD PHE A 286 43.159 22.723 125.657 1.00 32.55 ATOM 2281 C C PHE A 286 43.159 22.723 125.657 1.00 32.56 ATOM 2282 CD PHE A 286 43.159 22.723 125.657 1.00 32.56 ATOM 2282 CD PHE A 286 43.159 22.723 125.657 1.00 32.56 ATOM 2283 CD PHE A 286 43.159 22.723 125.657 1.00 32.56 ATOM 2283 C C PHE A 286 43.159 22.723 125.657 1.00 32.56 ATOM 2281 C C GLU A 288 45.461 1.381 24.991 122.202 1.00 32.96 ATOM 2281 C C GLU A 288 45.461 1.381 24.991 122.202 1.00 32.96 ATOM 2290 C | ATOM | 2256 | NE | ARG.A 28 | 3 | | | | | |
| ATOM 2259 NH1 ARG A 283 53.012 18.611 129.198 1.00 36.46 ATOM 2260 C ARG A 283 48.561 23.065 127.473 1.00 35.90 ATOM 2261 O ARG A 283 47.830 23.302 128.439 1.00 35.06 ATOM 2262 N GLU A 284 49.350 23.302 128.439 1.00 35.70 ATOM 2263 CA GLU A 284 49.350 23.302 128.439 1.00 35.70 ATOM 2264 CB GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2265 CG GLU A 284 50.499 26.166 126.799 1.00 60.69 ATOM 2266 CD GLU A 284 51.917 25.702 127.141 1.00 56.39 ATOM 2266 CD GLU A 284 53.012 27.778 126.542 1.00 60.69 ATOM 2267 CEI GLU A 284 53.810 25.880 125.680 1.00 62.79 ATOM 2269 C GLU A 284 53.810 25.880 125.680 1.00 62.79 ATOM 2269 C GLU A 284 47.525 26.783 127.954 1.00 38.52 ATOM 2270 C GLU A 284 47.525 26.783 127.954 1.00 38.52 ATOM 2271 N VAL A 285 46.039 26.291 124.062 1.00 33.75 ATOM 2271 C CA VAL A 285 46.039 26.291 124.062 1.00 35.43 ATOM 2277 C CB VAL A 285 46.039 26.291 124.062 1.00 36.43 ATOM 2277 C CB VAL A 285 44.654 26.811 123.693 1.00 37.26 ATOM 2277 C VAL A 285 44.654 26.811 123.693 1.00 37.57 ATOM 2276 C VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2277 C VAL A 285 44.694 25.688 126.611 1.00 41.83 ATOM 2277 C VAL A 285 44.694 25.688 126.611 1.00 41.83 ATOM 2277 C VAL A 285 44.694 25.688 126.611 1.00 37.26 ATOM 2277 C VAL A 285 44.694 25.688 126.611 1.00 36.96 ATOM 2278 N PHE A 286 43.760 23.360 126.611 1.00 31.95 ATOM 2228 C CD PHE A 286 43.760 23.499 122.255 1.00 33.95 ATOM 2228 C CD PHE A 286 43.760 23.499 122.255 1.00 33.95 ATOM 2280 C PHE A 286 43.760 23.499 122.255 1.00 33.95 ATOM 2280 C PHE A 286 43.760 23.499 122.255 1.00 33.96 ATOM 2280 C PHE A 286 43.760 23.499 122.255 1.00 33.96 ATOM 2280 C PHE A 286 43.760 23.499 122.255 1.00 33.96 ATOM 2280 C PHE A 286 43.760 23.499 122.255 1.00 33.96 ATOM 2280 C PHE A 286 43.760 23.499 122.255 1.00 33.96 ATOM 2280 C C PHE A 286 43.760 23.499 122.255 1.00 33.96 ATOM 2285 C C PHE A 286 43.760 23.499 122.255 1.00 33.96 ATOM 2285 C C PHE A 286 43.760 23.499 122.255 1.00 33.96 ATOM 2285 C C GLU A 288 46.910 17.864 133.1069 1.00 36.97 ATOM 2295 C C GLU A 288 46.910 17 | | | | | | | 18.351 | 129.742 | - | |
| ATOM 2260 C ARG A 283 | | | | | | | | | | |
| ATOM 2261 O ARG A 283 47.830 23.065 127.473 1.00 36.06 ATOM 2262 N GLU A 284 49.376 25.348 127.488 1.00 35.70 ATOM 2263 CA GLU A 284 49.376 25.348 127.488 1.00 40.93 ATOM 2264 CB GLU A 284 51.917 25.702 127.141 1.00 56.39 ATOM 2266 CD GLU A 284 51.917 25.702 127.141 1.00 56.39 ATOM 2266 CD GLU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2267 OE1 GLU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2268 OE2 GLU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2268 OE2 GLU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2269 C GLU A 284 48.039 26.014 127.148 1.00 39.24 ATOM 2270 O GLU A 284 47.525 26.783 127.954 1.00 33.75 ATOM 2271 N VAL A 285 46.205 26.294 125.592 1.00 33.75 ATOM 2273 CB VAL A 285 46.039 26.014 127.148 1.00 39.24 ATOM 2273 CB VAL A 285 46.039 26.024 127.954 1.00 33.75 ATOM 2273 CB VAL A 285 46.039 26.029 124.062 1.00 33.75 ATOM 2273 CG VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2276 C VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2277 O VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2278 N PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2278 N PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2278 N PHE A 286 43.760 23.608 126.753 1.00 35.96 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 33.96 ATOM 2281 CG PHE A 286 43.169 22.723 125.657 1.00 33.96 ATOM 2285 CP PHE A 286 44.931 24.919 122.419 1.00 31.67 ATOM 2285 CP PHE A 286 43.169 22.723 125.657 1.00 32.53 ATOM 2280 CB PHE A 286 44.931 24.919 122.419 1.00 31.67 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.16 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2280 CB PHE A 286 43.169 22.723 125.657 1.00 32.53 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.16 ATOM 2280 C CB PHE A 286 42.544 23.490 124.529 1.00 30.96 ATOM 2287 C PHE A 286 42.544 23.490 124.529 1.00 30.96 ATOM 2290 CA GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2290 C CB GLU A 288 45.613 17.57 | | | | | | | | | | |
| ATOM 2261 O ARG A 283 47.830 23.302 128.439 1.00 35.04 ATOM 2262 N GLU A 284 49.350 23.3085 126.928 1.00 35.70 ATOM 2263 CA GLU A 284 59.499 26.166 126.799 1.00 44.17 ATOM 2265 CG GLU A 284 59.499 26.166 126.799 1.00 44.17 ATOM 2266 CD GLU A 284 51.917 25.702 127.141 1.00 60.69 ATOM 2267 OEI GLU A 284 53.012 27.738 126.542 1.00 62.79 ATOM 2268 OEZ GLU A 284 53.012 27.738 126.542 1.00 62.79 ATOM 2269 C GLU A 284 48.039 26.014 127.148 1.00 39.51 ATOM 2269 C GLU A 284 48.039 26.014 127.148 1.00 39.55 ATOM 2271 N VAL A 285 47.472 25.704 127.195 1.00 38.52 ATOM 2271 N VAL A 285 46.039 26.291 124.062 1.00 38.52 ATOM 2272 CA VAL A 285 46.039 26.291 124.062 1.00 38.65 ATOM 2273 CB VAL A 285 46.039 26.291 124.062 1.00 34.14 ATOM 2273 CB VAL A 285 46.039 26.291 124.062 1.00 34.14 ATOM 2275 CG2 VAL A 285 44.654 26.811 123.693 1.00 37.57 ATOM 2276 C VAL A 285 44.964 25.638 125.992 1.00 34.14 ATOM 2275 CG2 VAL A 285 44.964 25.638 125.992 1.00 34.14 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 37.26 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 37.57 ATOM 2278 C PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2278 C PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2280 CB PHE A 286 44.931 24.308 126.235 1.00 35.05 ATOM 2281 CG PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2283 CD2 PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2283 CD2 PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2283 CD2 PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2280 CB PHE A 286 42.545 124.736 1.00 32.96 ATOM 2290 CB GLU A 288 45.613 17.576 131.663 1.00 37.57 ATOM 2290 CB GLU A 288 45.613 17.576 131 | | | | | | | | | | |
| ATOM 2263 CA GLU A 284 | | | | | | | | | | |
| ATOM 2264 CB GLU A 284 | | | | | | | | | | |
| ATOM 2266 CB GLU A 284 50.499 26.166 126.799 1.00 44.17 ATOM 2266 CD GLU A 284 51.917 25.702 127.141 1.00 60.69 ATOM 2267 OE1 GLU A 284 52.989 26.495 126.401 1.00 60.69 ATOM 2268 OE2 GLU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2269 CB GLU A 284 48.039 26.014 127.148 1.00 39.24 ATOM 2270 O GLU A 284 48.039 26.014 127.148 1.00 39.24 ATOM 2271 N VAL A 285 47.472 25.704 125.986 1.00 63.75 ATOM 2271 N VAL A 285 46.025 26.294 125.592 1.00 33.75 ATOM 2272 CA VAL A 285 46.025 26.294 125.592 1.00 33.75 ATOM 2273 CB VAL A 285 46.039 26.291 124.062 1.00 34.14 ATOM 2274 CG1 VAL A 285 44.654 26.681 123.419 1.00 38.58 ATOM 2275 CG2 VAL A 285 44.964 25.638 126.591 1.00 38.96 ATOM 2277 O VAL A 285 44.964 25.638 126.591 1.00 38.96 ATOM 2277 O VAL A 285 44.964 25.638 126.611 1.00 41.83 ATOM 2278 N PHE A 286 43.159 22.723 125.657 1.00 35.55 ATOM 2279 CA PHE A 286 43.159 22.723 125.657 1.00 35.55 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 30.15 ATOM 2281 CG PHE A 286 43.159 22.723 125.657 1.00 30.15 ATOM 2282 CD1 PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2283 CD2 PHE A 286 43.159 22.773 125.657 1.00 30.36 ATOM 2284 CE1 PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2285 CE2 PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2285 CE2 PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2285 CE2 PHE A 286 41.381 24.919 122.2419 1.00 31.66 ATOM 2285 CE2 PHE A 286 42.544 23.490 124.529 1.00 30.96 ATOM 2287 C PHE A 286 42.544 23.490 124.529 1.00 30.96 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.55 ATOM 2280 CB PHE A 286 42.544 23.490 124.529 1.00 30.55 ATOM 2280 CB PHE A 286 42.544 23.491 122.419 1.00 31.66 ATOM 2280 CB PHE A 286 42.544 23.491 122.202 1.00 30.06 ATOM 2280 CB PHE A 286 41.381 24.919 122.419 1.00 31.66 ATOM 2290 CA GLY 2 287 45.525 20.590 129.527 1.00 32.96 ATOM 2291 C GLY 3 288 45.646 18.273 130.310 1.00 32.54 ATOM 2292 CG GLY 3 288 46.910 17.864 132.411 1.00 45.36 ATOM 2293 CG GLU A 288 46. | | | | | | | | | | |
| ATOM 2265 CG GLU A 284 51.917 25.702 127.141 1.00 56.39 ATOM 2267 0E1 GLU A 284 52.989 26.495 126.401 1.00 60.69 ATOM 2268 0E2 GLU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2268 0E2 GLU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2270 0 GLU A 284 48.039 26.014 127.148 1.00 39.24 ATOM 2271 N VAL A 285 47.525 26.783 127.954 1.00 38.52 ATOM 2271 N VAL A 285 47.472 25.704 125.592 1.00 35.82 ATOM 2273 CB VAL A 285 46.039 26.291 124.062 1.00 34.14 ATOM 2273 CG VAL A 285 46.039 26.291 124.062 1.00 37.26 ATOM 2275 CG2 VAL A 285 44.654 26.811 123.693 1.00 37.26 ATOM 2276 C VAL A 285 44.964 25.638 126.192 1.00 37.26 ATOM 2277 O VAL A 285 44.964 25.638 126.611 1.00 41.83 ATOM 2278 N PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2279 CA PHE A 286 43.159 22.723 125.657 1.00 35.82 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 35.53 ATOM 2281 CG PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2282 CD PHE A 286 43.159 22.723 125.657 1.00 32.96 ATOM 2283 CD2 PHE A 286 43.159 22.723 125.657 1.00 32.96 ATOM 2284 CE1 PHE A 286 42.527 24.170 122.202 1.00 33.96 ATOM 2284 CE1 PHE A 286 40.813 24.958 123.693 1.00 31.67 ATOM 2286 C PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2287 C PHE A 286 40.813 24.958 123.693 1.00 31.67 ATOM 2288 O PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2289 C C PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2289 C C PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2289 C C PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2289 C C PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2289 C C PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2289 C C PHE A 286 40.813 24.958 123.693 1.00 31.67 ATOM 2289 C C C PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2289 C C C PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2289 C C C C PHE A 286 40.813 24.919 122.419 1.00 36.97 ATOM 2289 C C C C PHE A 286 42.527 1.00 122.20 1.00 32.96 ATOM 2290 C C GLU A 288 45.640 18.273 130.310 1.00 32.54 ATOM 2291 C GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2292 C C GLU A 288 48.910 17.864 132.411 1.00 45.36 ATOM 2293 N | | | | | | | | | | |
| ATOM 2266 CD GLU A 284 53.989 26.495 126.401 1.00 60.69 ATOM 2269 0E2 GLU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2269 C GLU A 284 48.039 26.014 127.148 1.00 38.52 ATOM 2270 O GLU A 284 47.525 26.783 127.954 1.00 38.52 ATOM 2271 N VAL A 285 47.472 25.704 125.986 1.00 33.75 ATOM 2271 CA VAL A 285 46.205 26.294 125.592 1.00 33.75 ATOM 2273 CB VAL A 285 46.025 26.294 125.592 1.00 34.14 ATOM 2273 CB VAL A 285 46.039 26.291 124.062 1.00 34.14 ATOM 2273 CG VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2275 CG2 VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2277 C VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2277 O VAL A 285 44.964 25.638 126.619 1.00 37.57 ATOM 2278 N PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2279 CA PHE A 286 43.760 23.608 126.753 1.00 35.05 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 30.15 ATOM 2281 CG PHE A 286 43.159 22.723 125.657 1.00 30.56 ATOM 2283 CD2 PHE A 286 43.104 23.459 124.529 1.00 33.96 ATOM 2283 CD2 PHE A 286 43.104 23.459 122.202 1.00 32.96 ATOM 2285 CE2 PHE A 286 43.104 23.459 122.202 1.00 32.96 ATOM 2285 CE2 PHE A 286 43.991 24.529 12.00 33.96 ATOM 2286 CP PHE A 286 42.547 24.170 122.202 1.00 32.96 ATOM 2286 CP PHE A 286 42.547 24.170 122.202 1.00 32.96 ATOM 2286 CP PHE A 286 43.992 22.773 128.015 1.00 33.96 ATOM 2286 CP PHE A 286 43.992 22.773 128.015 1.00 33.96 ATOM 2287 C PHE A 286 43.992 22.773 128.015 1.00 33.96 ATOM 2289 N GLY A 288 45.549 49.81 23.693 1.00 31.66 ATOM 2289 N GLY A 288 45.549 49.91 128.656 1.00 30.98 ATOM 2299 CA GLY 3.287 45.594 45.595 123.693 1.00 31.66 ATOM 2299 CA GLY 3.287 45.595 22.795 129.762 1.00 32.95 ATOM 2299 CB GLU A 288 45.691 17.864 132.411 1.00 45.65 ATOM 2299 OE2 GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2299 CB GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2299 OE2 GLU A 288 45.613 17.576 131.663 1.00 30.98 ATOM 2299 OE2 GLU A 288 45.613 17.576 131.663 1.00 30.98 ATOM 2303 CA GLU A 288 48.144 17.957 129.762 1.00 28.67 ATOM 2303 CA GLU A 288 48.144 17.957 129. | | | | | | | | | | |
| ATOM 2269 C GLU A 284 53.012 27.738 126.542 1.00 63.13 ATOM 2269 C GLU A 284 53.810 25.880 125.680 1.00 62.79 ATOM 2270 O GLU A 284 47.525 26.783 127.954 1.00 39.24 ATOM 2271 N VAL A 285 47.472 25.704 125.986 1.00 33.75 ATOM 2273 CB VAL A 285 46.205 26.294 125.592 1.00 35.82 ATOM 2273 CB VAL A 285 46.039 26.291 124.062 1.00 34.14 ATOM 2273 CB VAL A 285 46.039 26.291 124.062 1.00 34.14 ATOM 2275 CG2 VAL A 285 47.114 27.153 123.419 1.00 37.26 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 37.26 ATOM 2278 C VAL A 285 44.964 25.638 126.192 1.00 37.26 ATOM 2278 C VAL A 285 44.964 25.638 126.591 1.00 41.83 ATOM 2278 C PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2279 CA PHE A 286 43.159 22.723 125.657 1.00 35.53 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2281 CG PHE A 286 43.104 23.459 123.256 1.00 33.96 ATOM 2283 CD2 PHE A 286 43.104 23.459 123.256 1.00 33.96 ATOM 2283 CD2 PHE A 286 42.544 23.490 124.529 1.00 33.96 ATOM 2284 CE1 PHE A 286 42.547 24.170 122.202 1.00 32.96 ATOM 2285 CE2 PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2286 C PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2287 C PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2288 O PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2288 C PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2289 N GLY A 287 45.525 20.590 129.527 1.00 30.06 ATOM 2289 C G GLY A 288 45.464 18.273 130.310 1.00 32.53 ATOM 2299 C G GLY A 288 45.464 18.273 130.310 1.00 32.53 ATOM 2299 C C GLY A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2299 C C GLY A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2299 C C GLY A 288 45.644 18.273 130.310 1.00 32.93 ATOM 2299 C C GLY A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2299 C C GLY A 288 45.644 18.273 130.310 1.00 32.53 ATOM 2299 C C GLY A 288 48.144 17.957 129.762 1.00 30.96 ATOM 2299 C C GLY A 288 45.614 18.273 130.310 1.00 32.53 ATOM 2299 C C GLY A 288 48.144 17.957 129.762 1.00 30.98 ATOM 2299 C C GLY A 288 48.144 17.957 129.762 1.00 30.98 ATOM 2300 C G GLY A 288 48.144 17.957 129.762 1.00 30.98 ATOM 2301 C GLY A 289 44.6 | | | | | | | | | | |
| ATOM 2268 OE2 GLU A 284 | MOTA | | | | | | | | | |
| ATOM 2270 O GLU A 284 48.039 26.014 127.148 1.00 39.24 ATOM 2271 N VAL A 285 47.472 25.704 125.996 1.00 38.52 ATOM 2272 CA VAL A 285 46.039 26.291 125.592 1.00 35.82 ATOM 2273 CB VAL A 285 46.039 26.291 124.062 1.00 34.14 ATOM 2275 CG2 VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2275 CG2 VAL A 285 44.654 26.811 123.693 1.00 37.26 ATOM 2277 O VAL A 285 44.064 25.638 126.192 1.00 37.26 ATOM 2277 O VAL A 285 44.043 26.336 126.611 1.00 41.83 ATOM 2278 N PHE A 286 44.944 25.638 126.192 1.00 37.57 ATOM 2278 N PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2280 CB PHE A 286 43.760 23.608 126.753 1.00 35.05 ATOM 2281 CG PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2282 CD1 PHE A 286 42.544 23.490 124.529 1.00 30.35 ATOM 2283 CD2 PHE A 286 42.544 23.490 124.529 1.00 30.35 ATOM 2284 CD1 PHE A 286 42.544 23.490 124.529 1.00 30.35 ATOM 2286 CD PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2285 CE2 PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2286 CD PHE A 286 42.544 23.490 124.529 1.00 30.35 ATOM 2286 CD PHE A 286 42.544 23.490 124.529 1.00 30.36 ATOM 2287 C PHE A 286 42.544 23.490 122.202 1.00 30.30 ATOM 2286 CZ PHE A 286 42.544 23.490 122.202 1.00 30.30 ATOM 2287 C PHE A 286 42.544 23.490 122.202 1.00 30.30 ATOM 2288 O PHE A 286 42.544 23.490 122.202 1.00 30.30 ATOM 2286 CZ PHE A 286 42.544 23.490 122.202 1.00 30.96 ATOM 2287 C PHE A 286 42.544 23.490 122.202 1.00 30.96 ATOM 2289 C C GLY 2.287 45.525 20.590 129.527 1.00 34.44 ATOM 2290 CA GLY 2.287 45.525 20.590 129.527 1.00 34.44 ATOM 2291 C C GLY 2.287 45.525 20.590 129.527 1.00 34.44 ATOM 2292 C GLY 2.287 45.526 20.590 129.527 1.00 34.44 ATOM 2293 N GLU A 288 45.464 18.273 130.310 1.00 32.23 ATOM 2295 CB GLU A 288 45.464 18.273 130.310 1.00 32.53 ATOM 2295 CB GLU A 288 45.464 18.273 130.310 1.00 32.53 ATOM 2295 CB GLU A 288 45.464 18.273 130.310 1.00 32.53 ATOM 2295 CB GLU A 288 45.464 18.273 130.310 1.00 32.53 ATOM 2295 CB GLU A 288 45.464 18.273 130.310 1.00 32.53 ATOM 2299 CCD GLU A 288 44.404 17.455 131.663 1.00 45.36 ATOM 2299 CCD GLU A 288 44.404 17 | ATOM | 2267 | OE] | L GLU A 28 | 4 | 53.012 | .27.738 | 126.542 | 1.00 | 63.13 |
| ATOM 2270 O GLU A 284 47.525 26.783 127.954 1.00 38.52 ATOM 2271 N VAL A 285 47.472 25.704 125.986 1.00 33.75 ATOM 2272 CA VAL A 285 46.205 26.294 125.592 1.00 35.82 ATOM 2273 CB VAL A 285 46.039 26.291 124.062 1.00 34.14 ATOM 2275 CG2 VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2276 C VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2279 CA PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2279 CA PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2281 CG PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2283 CD2 PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2283 CD2 PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2283 CD2 PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2285 CE2 PHE A 286 42.544 23.490 122.202 1.00 32.96 ATOM 2285 CE2 PHE A 286 42.544 23.490 122.202 1.00 32.96 ATOM 2285 CE2 PHE A 286 42.544 23.490 122.202 1.00 33.96 ATOM 2287 CP PHE A 286 42.544 23.490 122.202 1.00 33.96 ATOM 2287 CP PHE A 286 42.544 29.91 122.419 1.00 31.66 ATOM 2287 CP PHE A 286 42.544 29.91 122.419 1.00 31.66 ATOM 2287 CP PHE A 286 42.544 29.91 122.419 1.00 31.66 ATOM 2289 N GLY A 287 45.086 22.840 128.403 1.00 35.18 ATOM 2290 CA GLY 7. 287 45.297 22.056 129.862 1.00 30.06 ATOM 2291 CP GLY 7. 287 45.525 20.590 129.527 1.00 34.44 ATOM 2292 CR GLY A 288 45.644 18.273 130.310 1.00 32.54 ATOM 2293 N GLU A 288 45.641 18.273 130.310 1.00 32.54 ATOM 2295 CB GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2295 CB GLU A 288 46.910 17.664 132.411 1.00 45.36 ATOM 2295 CB GLU A 288 46.910 17.664 132.411 1.00 45.36 ATOM 2299 CC2 GLU A 288 46.910 17.664 132.411 1.00 45.36 ATOM 2300 C GLU A 288 46.910 17.664 132.411 1.00 28.67 ATOM 2300 C GLU A 288 46.910 17.664 132.411 1.00 28.67 ATOM 2300 C GLU A 288 46.910 17.664 132.611 1.00 25.56 ATOM 2303 CA GLU A 289 44.614 16.694 128.657 1.00 28.67 ATOM 2303 CA GLU A 289 44.614 16.6 | ATOM | 2268 | OE2 | 2 GLU A 28 | 4 | 53.810 | 25.880 | 125.680 | 1.00 | 62.79 |
| ATOM 2271 N VAL A 285 47.472 25.704 125.986 1.00 33.75 ATOM 2272 CA VAL A 285 46.205 26.294 125.592 1.00 35.82 ATOM 2273 CB VAL A 285 46.205 26.294 125.592 1.00 34.14 ATOM 2274 CG1 VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2275 CG2 VAL A 285 44.664 26.811 123.693 1.00 36.43 ATOM 2277 C VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2278 N PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2279 CA PHE A 286 43.760 23.608 126.753 1.00 35.05 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 35.05 ATOM 2281 CG PHE A 286 43.159 22.723 125.657 1.00 35.05 ATOM 2282 CD1 PHE A 286 43.104 23.459 123.256 1.00 30.15 ATOM 2283 CD2 PHE A 286 43.104 23.459 123.256 1.00 30.30 ATOM 2284 CE1 PHE A 286 42.527 24.170 122.202 1.00 30.30 ATOM 2285 CE2 PHE A 286 42.527 24.170 122.202 1.00 30.30 ATOM 2286 CZ PHE A 286 40.813 24.958 123.693 1.00 31.67 ATOM 2286 CZ PHE A 286 43.922 22.773 128.015 1.00 35.18 ATOM 2288 O PHE A 286 43.922 22.773 128.015 1.00 35.18 ATOM 2289 N GLY A 287 45.984 22.080 128.409 1.00 30.87 ATOM 2290 CA GLY 287 45.525 20.590 129.527 1.00 34.44 ATOM 2291 C GLY 287 45.525 20.590 129.527 1.00 34.44 ATOM 2291 C GLY 287 45.525 20.590 129.527 1.00 34.44 ATOM 2292 O GLY 287 45.525 20.590 129.527 1.00 34.44 ATOM 2293 N GLU A 288 45.464 18.273 130.310 1.00 32.54 ATOM 2294 CA GLU A 288 45.588 19.710 130.500 1.00 28.42 ATOM 2297 CD GLU A 288 45.644 18.273 130.310 1.00 32.54 ATOM 2299 O GLU A 288 45.464 18.273 130.310 1.00 32.54 ATOM 2299 CG GLU A 288 46.910 17.455 131.663 1.00 37.03 ATOM 2299 CG GLU A 288 45.464 18.273 130.310 1.00 32.54 ATOM 2290 CG GLU A 288 46.910 17.664 132.665 1.00 30.98 ATOM 2300 C GLU A 288 46.910 17.663 132.666 1.00 30.98 ATOM 2300 C GLU A 288 48.140 17.455 131.662 1.00 30.98 ATOM 2300 C GLU A 288 48.140 17.455 131.663 1.00 37.92 ATOM 2300 C GLU A 288 48.140 17.957 129.762 1.00 28.67 ATOM 2300 C GLU A 288 43.144 17.957 129.762 1.00 28.67 ATOM 2300 C GLU A 288 43.144 17.957 129.762 1.00 28.67 ATOM 2300 C GLU A 288 43.1612 12.373 126.718 1.00 | ATOM | 2269 | С | GLU A 28 | 4 | 48.039 | 26.014 | 127.148 | 1.00 | 39.24 |
| ATOM 2271 N YAL A 285 47.472 25.704 125.986 1.00 33.75 ATOM 2272 CA VAL A 285 46.205 26.294 125.592 1.00 35.82 ATOM 2273 CB VAL A 285 46.039 26.291 124.062 1.00 34.14 ATOM 2274 CG1 VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2275 CG2 VAL A 285 44.664 26.811 123.693 1.00 36.43 ATOM 2276 C VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2278 N PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2279 CA PHE A 286 43.760 23.608 126.753 1.00 35.05 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2281 CG PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2282 CD1 PHE A 286 43.104 23.459 123.256 1.00 33.96 ATOM 2283 CD2 PHE A 286 43.104 23.459 123.256 1.00 33.96 ATOM 2284 CE1 PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2286 CE2 PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2286 CE2 PHE A 286 42.544 23.490 124.529 1.00 30.30 ATOM 2286 CE2 PHE A 286 42.547 24.710 122.202 1.00 32.96 ATOM 2286 CZ PHE A 286 42.87 24.91 124.91 1.00 31.67 ATOM 2286 CZ PHE A 286 43.81 24.958 123.693 1.00 31.67 ATOM 2288 O PHE A 286 43.922 22.773 128.015 1.00 35.18 ATOM 2289 N GLY A 287 45.894 22.080 128.409 1.00 36.97 ATOM 2290 CA GLY 287 45.525 20.590 129.527 1.00 34.44 ATOM 2291 C GLY 287 45.525 20.590 129.527 1.00 34.44 ATOM 2291 C GLY 287 45.525 20.590 129.527 1.00 34.44 ATOM 2292 O GLY A 288 45.464 18.273 130.310 1.00 32.54 ATOM 2293 N GLU A 288 45.914 20.264 128.403 1.00 32.54 ATOM 2294 CA GLU A 288 45.646 18.273 130.310 1.00 32.54 ATOM 2297 CD GLU A 288 46.910 17.864 132.09 1.00 45.65 ATOM 2299 O GLU A 288 45.641 16.334 131.069 1.00 45.36 ATOM 2290 CG GLU A 288 48.140 17.455 131.663 1.00 37.98 ATOM 2300 C GLU A 288 48.140 17.455 131.663 1.00 37.98 ATOM 2300 C GLU A 288 48.140 17.957 129.762 1.00 28.65 ATOM 2300 C GLU A 288 48.140 17.957 129.762 1.00 28.65 ATOM 2300 C GLU A 288 48.140 17.957 129.762 1.00 28.65 ATOM 2300 C GLU A 288 43.144 17.957 129.762 1.00 28.65 ATOM 2300 C GLU A 288 43.1612 12.373 126.718 1.00 25.90 ATOM 2300 C GLU A 288 43.622 14.510 127.866 1.00 | ATOM | 2270 | 0 | GLU A 28 | 4 | 47.525 | 26.783 | 127.954 | 1.00 | 38.52 |
| ATOM 2272 CA VAL A 285 46.205 26.294 125.592 1.00 35.82 ATOM 2274 CG1 VAL A 285 46.039 26.291 124.062 1.00 34.14 ATOM 2275 CG2 VAL A 285 44.654 26.811 123.693 1.00 36.43 ATOM 2276 C VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2277 O VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2278 N PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2279 CA PHE A 286 43.760 23.608 126.753 1.00 35.05 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2281 CG PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2282 CD1 PHE A 286 43.199 123.256 1.00 30.15 ATOM 2283 CD2 PHE A 286 41.398 24.245 124.736 1.00 30.30 ATOM 2284 CE1 PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2285 CE2 PHE A 286 41.398 24.245 124.736 1.00 31.66 ATOM 2286 CZ PHE A 286 43.922 22.773 128.015 1.00 31.66 ATOM 2287 C PHE A 286 43.922 22.773 128.015 1.00 33.96 ATOM 2288 O PHE A 286 42.984 22.080 128.409 1.00 36.87 ATOM 2289 N GLY A 287 45.984 128.695 1.00 30.87 ATOM 2290 CA GLY : 287 45.297 22.056 129.862 1.00 30.87 ATOM 2291 C GLY : 287 45.525 20.590 129.527 1.00 34.44 ATOM 2293 N GLU A 288 45.613 17.576 131.663 1.00 32.54 ATOM 2293 N GLU A 288 45.613 17.576 131.663 1.00 32.54 ATOM 2297 CD GLY : 287 45.525 20.590 129.527 1.00 34.44 ATOM 2298 OEI GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2297 CD GLU A 288 45.613 17.576 131.663 1.00 32.254 ATOM 2299 CB GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2299 CC GLU A 288 48.140 17.455 131.622 1.00 30.98 ATOM 2299 CC GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2300 C GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2301 O GLU A 288 48.140 17.455 131.622 1.00 29.66 ATOM 2302 N GLY A 289 43.625 15.999 127.886 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2300 C GLU A 288 44.409 17.623 129.546 1.00 29.66 ATOM 2301 O GLU A 288 43.141 1.00 25.90 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2303 CA GLY A 289 43.621 12.373 126.718 1.00 25.90 ATOM 2305 | | 2271 | N | 'VAL A 28 | 5 | 47.472 | 25.704 | 125.986 | | |
| ATOM 2273 CB VAL A 285 | | | CA | | | 46.205 | | | | |
| ATOM 2274 CG1 VAL A 285 | | | | | | | | | | |
| ATOM 2275 CG2 VAL A 285 47.114 27.153 123.419 1.00 37.26 ATOM 2276 C VAL A 285 44.964 25.638 126.192 1.00 38.96 ATOM 2277 O VAL A 285 44.964 25.638 126.611 1.00 41.83 ATOM 2278 N PHE A 286 44.931 24.308 126.236 1.00 37.57 ATOM 2279 CA PHE A 286 43.760 23.608 126.753 1.00 35.05 ATOM 2280 CB PHE A 286 43.159 22.723 125.657 1.00 32.53 ATOM 2281 CG PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2282 CD1 PHE A 286 42.544 23.490 124.529 1.00 30.15 ATOM 2283 CD2 PHE A 286 41.398 24.245 124.736 1.00 30.30 ATOM 2284 CE1 PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2285 CE2 PHE A 286 40.813 24.958 123.693 1.00 31.67 ATOM 2286 CZ PHE A 286 41.398 24.245 124.736 1.00 30.30 ATOM 2287 C PHE A 286 41.381 24.919 122.419 1.00 31.67 ATOM 2288 O PHE A 286 43.922 22.773 128.015 1.00 35.18 ATOM 2289 N GLY A 287 45.086 22.840 128.693 1.00 36.97 ATOM 2289 N GLY A 287 45.086 22.840 128.695 1.00 30.87 ATOM 2290 CA GLY 7.287 45.525 20.590 129.527 1.00 32.96 ATOM 2291 C GLY 7.287 45.927 22.056 129.862 1.00 30.06 ATOM 2291 C GLY 7.287 45.914 20.264 128.403 1.00 32.54 ATOM 2292 C GLU A 288 45.643 17.576 131.663 1.00 32.54 ATOM 2295 CB GLU A 288 45.643 17.576 131.663 1.00 32.53 ATOM 2299 OC2 GLU A 288 45.613 17.576 131.663 1.00 32.53 ATOM 2299 OC2 GLU A 288 45.613 17.576 131.663 1.00 32.23 ATOM 2299 OC2 GLU A 288 48.144 16.334 131.069 1.00 45.56 ATOM 2299 OC2 GLU A 288 48.144 16.334 131.069 1.00 45.56 ATOM 2300 C GLU A 288 48.144 16.334 131.069 1.00 45.56 ATOM 2300 C GLU A 288 43.144 17.577 129.762 1.00 28.67 ATOM 2301 O GLU A 288 43.144 17.577 129.762 1.00 29.66 ATOM 2302 N GLY A 289 43.625 15.999 127.886 1.00 30.98 ATOM 2303 CA GLY A 289 43.625 15.999 127.866 1.00 30.98 ATOM 2301 O GLU A 288 43.144 17.577 129.762 1.00 28.67 ATOM 2305 O GLY A 289 43.625 15.999 127.866 1.00 28.67 ATOM 2305 O GLY A 289 43.625 15.999 127.866 1.00 28.67 ATOM 2305 O GLY A 289 43.625 15.999 127.866 1.00 28.67 ATOM 2305 O GLY A 289 43.625 15.999 127.866 1.00 28.68 ATOM 2305 O GLY A 289 43.625 15.999 127.866 1.00 25.90 ATOM 2306 CB VAL A 290 44.681 14.007 128. | | | | | | | | | | |
| ATOM 2276 C VAL A 285 | | | | | | | | | | |
| ATOM 2277 O VAL A 285 | - | | | | | | | | | |
| ATOM 2278 N PHE A 286 | | | | | | | | | | |
| ATOM 2280 CB PHE A 286 | | | | | | | | | | |
| ATOM 2280 CB PHE A 286 | | | | | | | | | | |
| ATOM 2281 CG PHE A 286 | | | | | | | | | | |
| ATOM 2282 CD1 PHE A 286 43.104 23.459 123.256 1.00 33.96 ATOM 2283 CD2 PHE A 286 41.398 24.245 124.736 1.00 30.30 ATOM 2284 CE1 PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2285 CE2 PHE A 286 40.813 24.958 123.693 1.00 31.67 ATOM 2286 CZ PHE A 286 41.381 24.919 122.419 1.00 31.66 ATOM 2287 C PHE A 286 43.922 22.773 128.015 1.00 35.18 ATOM 2288 O PHE A 286 42.984 22.080 128.409 1.00 36.97 ATOM 2289 N GLY A 287 45.086 22.840 128.656 1.00 30.87 ATOM 2290 CA GLY 7.287 45.297 22.056 129.862 1.00 30.06 ATOM 2291 C GLY 7.287 45.525 20.590 129.527 1.00 34.44 ATOM 2292 O GLY 7.287 45.525 20.590 129.527 1.00 34.44 ATOM 2292 O GLY 7.287 45.914 20.264 128.403 1.00 32.54 ATOM 2293 N GLU A 288 45.288 19.710 130.500 1.00 28.42 ATOM 2295 CB GLU A 288 45.464 18.273 130.310 1.00 32.23 ATOM 2295 CB GLU A 288 45.6613 17.576 131.663 1.00 37.02 ATOM 2296 CG GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2299 OE2 GLU A 288 48.144 16.334 131.069 1.00 45.46 ATOM 2299 OE2 GLU A 288 48.144 16.334 131.069 1.00 46.42 ATOM 2299 OE2 GLU A 288 48.144 16.334 131.069 1.00 46.42 ATOM 2300 C GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2300 C GLU A 288 43.144 17.957 129.762 1.00 28.67 ATOM 2301 O GLU A 288 43.144 17.957 129.762 1.00 28.67 ATOM 2302 N GLY A 289 43.625 15.999 127.886 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 25.90 ATOM 2304 C GLY A 289 43.625 15.999 127.886 1.00 25.36 ATOM 2305 O GLY A 289 43.625 15.999 127.886 1.00 25.36 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 25.36 ATOM 2308 CB VAL A 290 43.384 13.807 126.868 1.00 25.36 ATOM 2308 CB VAL A 290 43.384 13.807 126.868 1.00 25.36 ATOM 2309 CG1 VAL A 290 43.384 13.807 126.664 1.00 25.36 ATOM 2309 CG1 VAL A 290 43.5612 1.2373 126.618 1.00 25.36 ATOM 2309 CG1 VAL A 290 43.5612 1.2373 126.618 1.00 25.36 ATOM 2309 CG1 VAL A 290 43.5612 1.2373 126.618 1.00 25.36 ATOM 2309 CG1 VAL A 290 43.5612 1.0148 126.664 1.00 25.36 ATOM 2309 CG1 VAL A 290 43.5612 1.0148 126.664 1.00 25.36 ATOM 2309 CG1 VAL A 290 4 | | | | | | | | | | |
| ATOM 2283 CD2 PHE A 286 41.398 24.245 124.736 1.00 30.30 ATOM 2284 CE1 PHE A 286 42.527 24.170 122.202 1.00 32.96 ATOM 2285 CE2 PHE A 286 40.813 24.958 123.693 1.00 31.67 ATOM 2286 CZ PHE A 286 41.381 24.958 123.693 1.00 31.67 ATOM 2287 C PHE A 286 41.381 24.958 123.693 1.00 31.67 ATOM 2287 C PHE A 286 43.922 22.773 128.015 1.00 35.18 ATOM 2288 O PHE A 286 42.984 22.080 128.409 1.00 36.97 ATOM 2289 N GLY A 287 45.086 22.840 128.656 1.00 30.87 ATOM 2290 CA GLY 287 45.297 20.566 129.862 1.00 30.06 ATOM 2291 C GLY 287 45.525 20.550 129.527 1.00 34.44 ATOM 2292 O GLY 287 45.525 20.550 129.527 1.00 34.44 ATOM 2293 N GLU A 288 45.288 19.710 130.500 1.00 28.42 ATOM 2294 CA GLU A 288 45.464 18.273 130.310 1.00 32.23 ATOM 2295 CB GLU A 288 45.464 18.273 130.310 1.00 32.23 ATOM 2296 CG GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2296 CG GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2297 CD GLU A 288 48.140 17.455 131.662 1.00 45.65 ATOM 2299 OE2 GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2300 C GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2301 O GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2301 O GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2302 N GLY A 289 44.641 16.634 129.565 1.00 28.67 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 44.641 16.694 128.657 1.00 25.90 ATOM 2305 O GLY A 289 44.661 14.007 128.739 1.00 25.90 ATOM 2307 CA VAL A 290 43.384 14.007 128.739 1.00 25.90 ATOM 2307 CA VAL A 290 43.384 14.007 128.739 1.00 25.90 ATOM 2308 CB VAL A 290 43.384 11.626 126.412 1.00 25.36 ATOM 2309 CG1 VAL A 290 42.288 11.626 126.412 1.00 25.36 ATOM 2309 CG1 VAL A 290 42.288 11.626 126.412 1.00 25.36 ATOM 2309 CG1 VAL A 290 42.288 11.626 126.412 1.00 25.36 ATOM 2309 CG1 VAL A 290 42.288 11.626 126.412 1.00 25.36 ATOM 2309 CG1 VAL A 290 42.288 11.626 126.412 1.00 25.36 ATOM 2309 CG1 VAL A 290 42.288 11.626 126.412 1.00 25.36 ATOM 2309 CG1 VAL A 290 42.288 11.626 126.412 1.00 25.36 ATOM 2309 CG1 VAL A 290 42.288 11.626 126.412 1.00 25.36 ATOM 2309 CG1 VAL A 290 42.288 11.626 | | | | | | | | | | |
| ATOM 2284 CE1 PHE A 286 | | | | | | | | | | |
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| ATOM 2286 CZ PHE A 286 41.381 24.919 122.419 1.00 31.66 ATOM 2287 C PHE A 286 43.922 22.773 128.015 1.00 35.18 ATOM 2288 O PHE A 286 42.984 22.080 128.409 1.00 36.97 ATOM 2289 N GLY A 287 45.086 22.840 128.656 1.00 30.87 ATOM 2290 CA GLY : 287 45.525 20.590 129.527 1.00 34.44 ATOM 2291 C GLY : 287 45.525 20.590 129.527 1.00 34.44 ATOM 2292 O GLY : 287 45.914 20.264 128.403 1.00 32.54 ATOM 2293 N GLU A 288 45.464 18.273 130.310 1.00 32.54 ATOM 2295 CB GLU A 288 45.464 18.273 130.310 1.00 32.23 ATOM 2295 CB GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2297 CD GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2297 CD GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2299 OE2 GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2300 C GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2300 C GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2301 O GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 28.67 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.67 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.67 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.68 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 43.625 15.999 127.886 1.00 25.90 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2308 CB VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2309 CG1 VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATOM 2287 C PHE A 286 43.922 22.773 128.015 1.00 35.18 ATOM 2288 O PHE A 286 42.984 22.080 128.409 1.00 36.97 ATOM 2289 N GLY A 287 45.086 22.840 128.656 1.00 30.87 ATOM 2290 CA GLY : 287 45.297 22.056 129.862 1.00 30.06 ATOM 2291 C GLY : 287 45.525 20.590 129.527 1.00 34.44 ATOM 2292 O GLY : 287 45.525 20.590 129.527 1.00 34.44 ATOM 2293 N GLU A 288 45.914 20.264 128.403 1.00 32.54 ATOM 2294 CA GLU A 288 45.464 18.273 130.310 1.00 32.23 ATOM 2295 CB GLU A 288 45.464 18.273 130.310 1.00 32.23 ATOM 2296 CG GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2297 CD GLU A 288 48.140 17.455 131.662 1.00 45.65 ATOM 2298 OE1 GLU A 288 48.140 17.455 131.662 1.00 45.65 ATOM 2299 OE2 GLU A 288 48.140 17.455 131.662 1.00 46.42 ATOM 2300 C GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2301 O GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 28.67 ATOM 2302 N GLY A 289 43.625 15.999 127.886 1.00 28.67 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.67 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.67 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.67 ATOM 2305 O GLY A 289 43.625 15.999 127.886 1.00 28.67 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 25.90 ATOM 2307 CA VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2308 CB VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATOM 2288 O PHE A 286 42.984 22.080 128.409 1.00 36.97 ATOM 2289 N GLY A 287 45.086 22.840 128.656 1.00 30.87 ATOM 2290 CA GLY 7.287 45.297 22.056 129.862 1.00 30.06 ATOM 2291 C GLY 1.287 45.525 20.590 129.527 1.00 34.44 ATOM 2292 O GLY 7.287 45.914 20.264 128.403 1.00 32.54 ATOM 2293 N GLU A 288 45.288 19.710 130.500 1.00 28.42 ATOM 2294 CA GLU A 288 45.464 18.273 130.310 1.00 32.23 ATOM 2295 CB GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2296 CG GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2297 CD GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2299 OE2 GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2299 OE2 GLU A 288 48.140 17.455 131.691 1.00 50.78 ATOM 2300 C GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2301 O GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 43.625 15.999 127.886 1.00 25.90 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.384 13.807 126.868 1.00 26.53 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.288 11.626 126.412 1.00 25.36 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATOM 2289 N GLY A 287 | atom | | | | | | | | | |
| ATOM 2290 CA GLY : 287 | | | | | | | | | | |
| ATOM 2291 C- GLY : 287 | MOTA | 2289 | N | | | | | | | |
| ATOM 2292 O GLY 7. 287 45.914 20.264 128.403 1.00 32.54 ATOM 2293 N GLU A 288 45.288 19.710 130.500 1.00 28.42 ATOM 2294 CA GLU A 288 45.464 18.273 130.310 1.00 32.23 ATOM 2295 CB GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2296 CG GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2297 CD GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2298 OE1 GLU A 288 48.140 17.655 131.622 1.00 45.65 ATOM 2299 OE2 GLU A 288 48.144 16.334 131.069 1.00 46.42 ATOM 2300 C GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2301 O GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 28.67 ATOM 2303 CA GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2304 C GLY A 289 43.625 15.999 127.861 1.00 28.08 ATOM 2305 O GLY A 289 43.625 15.999 127.861 1.00 25.90 ATOM 2305 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.384 13.807 126.868 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | ATOM | 2290 | CA | | | | 22.056 | 129.862 | 1.00 | 30.06 |
| ATOM 2293 N GLU A 288 45.288 19.710 130.500 1.00 28.42 ATOM 2294 CA GLU A 288 45.464 18.273 130.310 1.00 32.23 ATOM 2295 CB GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2296 CG GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2297 CD GLU A 288 48.140 17.455 131.662 1.00 45.65 ATOM 2298 OE1 GLU A 288 48.144 16.334 131.069 1.00 46.42 ATOM 2299 OE2 GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2300 C GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2301 O GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 28.67 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2304 C GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 43.625 15.999 127.861 1.00 30.45 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.384 13.807 126.868 1.00 27.31 ATOM 2308 CB VAL A 290 42.554 10.148 126.204 1.00 25.36 | ATOM | 2291 | C- | GLY : 28 | 7 | 45.525 | 20.590 | 129.527 | 1.00 | 34.44 |
| ATOM 2294 CA GLU A 288 45.464 18.273 130.310 1.00 32.23 ATOM 2295 CB GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2296 CG GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2297 CD GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2299 OE2 GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2299 OE2 GLU A 288 48.144 16.334 131.069 1.00 46.42 ATOM 2300 C GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2301 O GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 28.67 ATOM 2303 CA GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 44.618 14.510 127.861 1.00 30.45 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | ATOM | 2292 | 0 | GLY 7. 28 | 7 | 45.914 | 20.264 | 128.403 | 1.00 | 32.54 |
| ATOM 2295 CB GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2296 CG GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2297 CD GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2298 OE1 GLU A 288 48.144 16.334 131.069 1.00 46.42 ATOM 2299 OE2 GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2300 C GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2301 O GLU A 288 43.144 17.957 129.762 1.00 28.67 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2304 C GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 44.618 14.007 128.739 1.00 25.90 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | MOTA | 2293 | N | GLU A 28 | 3 · | 45.288 | 19.710 | 130.500 | 1.00 | 28.42 |
| ATOM 2295 CB GLU A 288 45.613 17.576 131.663 1.00 37.02 ATOM 2296 CG GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2297 CD GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2298 OE1 GLU A 288 48.144 16.334 131.069 1.00 46.42 ATOM 2299 OE2 GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2300 C GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2301 O GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 28.67 ATOM 2303 CA GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 44.618 14.510 127.861 1.00 30.45 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | ATOM | 2294 | CA | GLU A 28 | 3 | 45.464 | 18.273 | 130.310 | 1.00 | 32.23 |
| ATOM 2296 CG GLU A 288 46.910 17.864 132.411 1.00 45.36 ATOM 2297 CD GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2298 OE1 GLU A 288 48.144 16.334 131.069 1.00 46.42 ATOM 2299 OE2 GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2300 C GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2301 O GLU A 288 43.144 17.957 129.762 1.00 28.67 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.866 1.00 28.08 ATOM 2304 C GLY A 289 43.625 15.999 127.866 1.00 28.08 ATOM 2305 O GLY A 289 43.625 15.999 127.866 1.00 28.08 ATOM 2305 O GLY A 289 44.618 14.007 128.739 1.00 25.90 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2309 CG1 VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | ATOM | 2295 | CB | GLU A 28 | 3 | 45.613 | 17.576 | 131.663 | 1.00 | 37.02 |
| ATOM 2297 CD GLU A 288 48.140 17.455 131.622 1.00 45.65 ATOM 2298 OE1 GLU A 288 48.144 16.334 131.069 1.00 46.42 ATOM 2299 OE2 GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2300 C GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2301 O GLU A 288 43.144 17.957 129.762 1.00 28.67 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2304 C GLY A 289 43.922 14.510 127.861 1.00 30.45 ATOM 2305 O GLY A 289 44.618 14.007 128.739 1.00 25.90 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | 2296 | CG | GLU A 289 | 3 | 46.910 | 17.864 | 132.411 | 1.00 | 45.36 |
| ATOM 2298 OE1 GLU A 288 48.144 16.334 131.069 1.00 46.42 ATOM 2299 OE2 GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2300 C GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2301 O GLU A 288 43.144 17.957 129.762 1.00 28.67 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2304 C GLY A 289 43.922 14.510 127.861 1.00 30.45 ATOM 2305 O GLY A 289 44.618 14.307 128.739 1.00 25.90 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATOM 2300 C GLU A 288 49.106 18.245 131.571 1.00 50.78 ATOM 2301 O GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2301 O GLU A 288 43.144 17.957 129.762 1.00 28.67 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2304 C GLY A 289 43.625 15.999 127.861 1.00 30.45 ATOM 2305 O GLY A 289 43.922 14.510 127.861 1.00 30.45 ATOM 2305 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATOM 2300 C GLU A 288 44.309 17.623 129.546 1.00 30.98 ATOM 2301 O GLU A 288 43.144 17.957 129.762 1.00 28.67 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2304 C GLY A 289 43.922 14.501 127.861 1.00 30.45 ATOM 2305 O GLY A 289 44.618 14.007 128.739 1.00 25.90 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATOM 2301 O GLU A 288 43.144 17.957 129.762 1.00 28.67 ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2305 O GLY A 289 44.618 14.510 127.861 1.00 30.45 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 25.90 ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATOM 2302 N GLY A 289 44.641 16.694 128.657 1.00 29.66 ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2304 C GLY A 289 43.922 14.510 127.861 1.00 30.45 ATOM 2305 N VAL A 290 43.384 13.807 126.868 1.00 25.90 ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATOM 2303 CA GLY A 289 43.625 15.999 127.886 1.00 28.08 ATOM 2304 C GLY A 289 43.922 14.510 127.861 1.00 30.45 ATOM 2305 O GLY A 289 44.618 14.007 128.739 1.00 25.90 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATOM 2304 C GLY A 289 43.922 14.510 127.861 1.00 30.45 ATOM 2305 O GLY A 289 44.618 14.007 128.739 1.00 25.90 ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATCM 2305 O GLY A 289 44.618 14.007 128.739 1.00 25.90 ATCM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATCM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATCM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATCM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATOM 2306 N VAL A 290 43.384 13.807 126.868 1.00 26.21 ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | | | | | | | | | |
| ATOM 2307 CA VAL A 290 43.612 12.373 126.718 1.00 27.31 ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | ATOM | | | | | | 14.307 | 128.739 | | |
| ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | ATOM | | | | | | 13.807 | 126.868 | | |
| ATOM 2308 CB VAL A 290 42.288 11.626 126.412 1.00 26.53 ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | ATOM | 2307 | CA | | | | 12.373 | 126.718 | | |
| ATOM 2309 CG1 VAL A 290 42.554 10.148 126.204 1.00 25.36 | | 2308 | | | | | 11.626 | 126.412 | | |
| > 000 | | 2309 | CG1 | VAL A 290 |) | | 10.148 | 126.204 | | |
| | | 2310 | CG2 | VAL A 290 |) | 41.308 | 11.822 | 127.565 | 1.00 | 24.38 |

| ATO | M 2311 C VAL A 290 | 44.580 | 0 12.248 125.550 1.00 24.55 |
|--------------|--|---------------------------|--|
| ATO | M 2312 O VAL A 290 | 44.30 | |
| ATO | M 2313 N TYR A 291 | 45.716 | |
| ATO | | 46.729 | 1 11 10 10 1 |
| ATO | | 48.092 | |
| OTA | | 48.040 | 11.817 125.342 1.00 18.40 13.113 126.118 1.00 21.60 |
| ATO | 4 2317 CD1 TYR A 291 | 48.326 | |
| aton | 1 2318 CE1 TYR A 291 | 48.200 | 1.00 23.83 |
| ATOM | | 47.634 | 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| ATOR | 1 2320 CE2 TYR A 291 | 47.504 | |
| ATOM | | 47.786 | 1.00 ZO 1 |
| ATOM | | 47.631 | |
| ATOM | | 46.768 | |
| ATOM | 224 | 46.837 | |
| ATOM | | 46.755 | |
| ATOM | 252 | 46.767 | 8.924 121.902 1.00 20.69 |
| ATOM | | 45.482 | 8.842 121.076 1.00 22.13 |
| ATOM | | 44.162 | 9.063 121.814 1.00 23.78 |
| MOTA | | 43.001 | 8.959 120.826 1.00 23.09 |
| ATOM | | 44.008 | 8.050 122.930 1.00 16.01 |
| ATOM | | 47.953 | 8.885 120.947 1.00 22.90 |
| ATOM | 11 272 | 48.527 | 9.923 120.617 1.00 22.31 |
| ATOM | 2,3 | 48.301 | 7.684 120.491 1.00 18.83 |
| ATOM | 2334 CA GLY A 293 | 49.401 | 7.529 119.554 1.00 24.35 |
| ATOM | 2335 C GLY A 293 | 48.908 | 7.846 118.154 1.00 24.22 |
| ATOM | 2336 O GLY A 293 | 48.025 | 8.684 117.991 1.00 20 46 |
| ATOM | 2337 N GLY A 294 | 49.459 | 7.177 117.148 1.00 24.63 |
| ATOM | 2338 CA GLY A 294 | 49.035 | 7.423 115.779 1.00 22.03 |
| ATOM ATOM | 2339 C GLY A 294 | 50.024 | 6.869 114.769 1.00 22 90 |
| ATOM | 2340 O GLY A 294 2341 N GLY A 295 | 50.956 | 6.150 115.136 1.00 24.10 |
| MOTA | | 49.825 | 7.203 113.499 1.00 19.85 |
| ATOM | 2342 CA GLY A 295 2343 C GLY A 295 | 50.721 | 6.724 112.458 1.00 23.33 |
| ATOM | 2244 0 0 0 | 52.185 | 7.010 112.740 1.00 19.01 |
| ATOM | 2344 O GLY A 295 . 2345 N GLY A 296 | 52.541 | 8.094 113.196 1.00 19.39 |
| ATOM | 2346 CA GLY A 296 | 53.035 | 6.026 112.472 1.00 25.85 |
| ATOM | 2347 C GLY A 296 | 54.468 | 6.162 112.690 1.00 22.65 |
| ATOM | 2348 O GLY A 296 | 55.098 54.7 7 8 | 4.898 112.146 1.00 25.31 |
| ATOM | 2349 N TYR A 297 | 56.005 | 3.798 112.609 1.00 25.86 |
| ATOM | 2350 CA TYR A 297 | 56.598 | 5.034 111.185 1.00 22.83 3.852 110.577 1.00 23 93 |
| ATOM | 2351 CB TYR A 297 | 56.137 | |
| ATOM | 2352 CG TYR A 297 | 54.660 | |
| ATOM | 2353 CD1 TYR A 297 | 54.203 | 2:00 25:05 |
| ATOM | 2354 CE1 TYR A 297 | 52.842 | |
| ATOM | 2355 CD2 TYR A 297 | 53.713 | |
| ATOM | 2356 CE2 TYR A 297 | 52.352 | 3.062 109.116 1.00 25.28 3.346 109.190 1.00 21.83 |
| ATOM | 2357 CZ TYR A 297 | 51.927 | 4.666 109.181 1.00 21.81 |
| ATOM | 2358 OH TYR A 297 | 50.588 | 4.972 109.305 1.00 19.51 |
| ATOM | 2359 C TYR A 297 | 58.104 | 3.694 110.674 1.00 23.78 |
| -TOM | 2360 O TYR A 297 | 58.665 | 2.724 110.154 1.00 22.07 |
| ATOM | 2361 N HIS A 298 | 58.765 | 4.641 111.326 1.00 23.71 |
| ATOM | 2362 CA HIS A 298 | 60.204 | 4.534 111.517 1.00 26.33 |
| ATOM | 2363 CB HIS A 298 | 60.913 | 5.852 111.216 1.00 28.74 |
| ATOM | 2364 CG HIS A 298 | 62.403 | 5.727 111.213 1.00 33.08 |
| ATOM | 2365 CD2 HIS A 298 | 63.273 | 5.465 112.215 1.00 31.83 |
| ATOM | 2366 ND1 HIS A 298 | 63.151 | 5.775 110.056 1.00 32.49 |
| ATOM | 2367 CE1 HIS A 298 | 64.419 | .5.547 110.345 1.00 29.10 |
| ATCM | 2368 NE2 HIS A 298 | 64.520 | 5.354 111.648 1.00 38.70 |
| ATOM | 2369 C HIS A 298 | 60.371 | 4.188 112.996 1.00 27.81 |
| ATOM | 2370 O HIS A 298 | 60.120 | 5.020 113.865 1.0C 25.07 |
| ATOM | 2371 N PRO A 299 | 60.829 | 2.963 113.297 1.00 29.37 |
| ATOM | 2372 CD PRO A 299 | 61.285 | 1.932 112.352 1.00 26.09 |
| ATOM | 2373 CA PRO A 299 | 61.024 | 2.491 114.669 1.00 29.46 |
| ATOM | 2374 CB PRO A 299 | 61.675 | 1.118 114.465 1.00 29.03 |
| TOM | 2375 CG PRO A 299 2376 C PRO A 299 | 62.411 | 1.306 113.137 1.00 27.34 |
| ATOM . | C PRU A 233 | 61.849 | 3.403 115.570 1.00 31.88 |
| | | | |

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Figure 18-37

| ATOM | 2377 | 7 O PROA 299 | 61.480 | 3.622 116.724 | 1.00 32.45 |
|------|-------|---------------|----------------|----------------|------------|
| ATOM | 2378 | | 62.959 | | |
| MOTA | 2379 | | 63.803 | | |
| ATOM | 2380 | | | | 1.00 27.34 |
| | | | 65.163 | 5.058 115.207 | 1.00 26.84 |
| ATOM | 2381 | | 65.912 | 3.821 114.738 | 1.00 29.09 |
| MOTA | 2382 | CD1 TYR A 300 | 65.517 | 2.539 115.120 | 1.00 30.93 |
| ATOM | 2383 | CE1 TYR A 300 | 66.214 | 1.411 114.682 | 1.00 30.68 |
| ATOM | 2384 | | 67.027 | 3.941 113.908 | 1.00 29.72 |
| ATOM | 2385 | | | | 1.00 29.72 |
| | | | 67.730 | 2.829 113.466 | 1.00 30.76 |
| MOTA | 2386 | | 67.320 | 1.568 113.854 | 1.00 33.89 |
| ATOM | 2387 | | 68.011 | 0.471 113.404 | 1.00 34.70 |
| MOTA | 2388 | C TYR A 300 | 63.113 | 6.134 116.137 | 1.00 23.44 |
| ATOM | 2389 | O TYR A 300 | 63.108 | 6.631 117.264 | 1.00 23.87 |
| ATOM | 2390 | | 62.530 | 6.711 115.092 | |
| ATOM | 2391 | | 61.839 | 7 003 115 316 | 1.00 22.19 |
| - | 2392 | | | 7.993 115.216 | 1.00 26.50 |
| ATOM | | | 61.266 | 8.416 113.864 | 1.00 24.16 |
| ATOM | 2393 | | 60.715 | 7.878 116.237 | 1.00 27.86 |
| ATOM | 2394 | O ALA A 301 | 60.556 | 8.728 117.117 | 1.00 22.47 |
| ATOM | -2395 | N LEU A 302 | 59.940 | 6.808 116.110 | 1.00 23.27 |
| ATOM | 2396 | CA LEU A 302 | 58.818 | 6.566 116.996 | 1.00 26.50 |
| ATOM | 2397 | CB LEU A 302 | 58.036 | | 1.00 26.30 |
| | | | | 5.354 116.483 | 1.00 26.02 |
| ATOM | 2398 | CG LEU A 302 | 56.866 | 4.798 117.291 | 1.00 29.73 |
| ATOM | 2399 | CD1 LEU A 302 | 55.983 | 3.938 116.394 | 1.00 31.01 |
| ATOM | 2400 | CD2 LEU A 302 | 57.394 | 4.001 118.465 | 1.00 32.99 |
| MOTA | 2401 | C LEU A 302 | 59.246 | 6.373 118.451 | 1.00 27.49 |
| ATOM | 2402 | O LEU A 302 | 58.648 | 6.946 119.358 | 1.00 25.22 |
| ATOM | 2403 | N ALA A 303 | 60.289 | 5.580 118.672 | |
| ATOM | 2404 | CA ALA A 303 | 60.765 | | 1.00 27.85 |
| | 2405 | | | 5.320 120.024 | 1.00 27.33 |
| ATOM | | | 61.854 | 4.269 119.990 | 1.00 29.17 |
| MOTA | 2406 | C ALA A 303 | 61.27 9 | 6.580 120.714 | 1.00 26.64 |
| MOTA | 2407 | O ALA A 303 | . 60.944 | 6.849 121.875 | 1.00 23,18 |
| ATOM | 2408 | N ARG A 304 | 62.092 | 7.354 120.003 | 1.00 27.48 |
| ATOM | 2409 | CA ARG A 304 | 62.648 | 8.570 120.581 | 1.00 25.46 |
| ATOM | 2410 | CB ARG A 304 | 63.773 | 9.136 119.704 | 1.00 21.31 |
| ATOM | 2411 | CG ARG A 304 | 65 .005 | 8.231 119.562 | |
| | 2412 | CD ARG A 304 | | | 1.00 25.98 |
| ATOM | | | 66.153 | 9.042 118.951 | 1.00 27.87 |
| MOTA | 2413 | NE ARG A 304 | 65.647 | 9.766 117.796 | 1.00 36.76 |
| ATOM | 2414 | CZ ARG A 304 | 66.207 | 10.838 117.261 | 1.00 30.79 |
| MOTA | 2415 | NH1 ARG A 304 | 67.323 | 11.345 117.768 | 1.00 30.11 |
| ATOM | 2416 | NH2 ARG A 304 | 65.623 | 11.419 116.225 | 1.00 36.07 |
| ATOM | 2417 | C ARG A 304 | 61.585 | 9.634 120.803 | 1.00 25.46 |
| ATOM | 2418 | O ARG A 304 | 61.519 | 10.237 121.876 | 1.00 24.23 |
| ATOM | 2419 | N ALA A 305 | 60.741 | 9.854 119.802 | |
| | 2420 | | | | 1.00 22.22 |
| ATOM | | | 59.700 | 10.868 119.910 | 1.00 26.70 |
| ATOM | 2421 | CB ALA A 305 | 58.914 | 10.960 118.607 | 1.00 28.14 |
| MOTA | 2422 | C ALA A 305 | 58.749 | 10.626 121.072 | 1.00 25.54 |
| ATOM | 2423 | O ALA A 305 | 5 8 513 | 11.520 121.883 | 1.00 24.17 |
| ATOM | 2424 | N TRP A 306 | 58 1.89 | 9.426 121.160 | 1.00 25.66 |
| ATOM | 2425 | CA TRP A 306 | 57.270 | 9.157 122.253 | 1.00 28.01 |
| ATOM | 2426 | CB TRP A 306 | 56.454 | 7.873 122.012 | 1.00 18.66 |
| ATOM | 2427 | | | | |
| | | | 55.382 | 8.052 120.973 | 1.00 21.80 |
| ATOM | 2428 | CD2 TRP A 306 | 54.709 | 7.019 120.240 | 1.00 24.88 |
| MOTA | 2429 | CE2 TRP A 306 | 53.725 | 7.646 119.442 | 1.00 23.98 |
| ATOM | 2430 | CE3 TRP A 306 | 54.839 | 5.623 120.181 | 1.00 23.26 |
| MOTA | 2431 | CD1 TRP A 306 | 54.795 | 9.228 120.599 | 1.00 20.24 |
| ATOM | 2432 | NE1 TRP A 306 | 53.799 | 8.995 119.681 | 1.00 24.18 |
| ATOM | 2433 | CZ2 TRP A 306 | 52.875 | 6.926 118.590 | |
| | | CZ3 TRP A 306 | | | 1.00 24.30 |
| ATOM | 2434 | | 53.993 | 4.906 119.335 | 1.00 23.89 |
| ATOM | 2435 | CH2 TRP A 306 | 53.024 | 5.562 118.550 | 1.00 24.12 |
| MOTA | 2436 | C TRP A 306 | 57.969 | 9.113 123.605 | 1.00 27.93 |
| ATOM | 2437 | O TRP A 306 | 57.330 | 9.319 124.637 | 1.00 28.58 |
| ATOM | 2438 | N THR A 307 | 59.273 | 8.851 123.615 | 1.00 26.76 |
| ATOM | 2439 | CA THR A 307 | 60.000 | 8.850 124.881 | 1.00 22.81 |
| | 2440 | CB THR A 307 | 61.457 | | |
| ATOM | | | | 8.319 124.730 | 1.00 25.54 |
| ATOM | 2441 | OG1 THR A 307 | 61.435 | 6.902 124.504 | 1.00 22.73 |
| MOTA | 2442 | CG2 THR A 307 | 62.269 | 8.599 125.988 | 1.00 24.03 |

| ATOM | 2443 C THR A 307 | 60.027 | 7 10.288 125.39 | 5 1.00 26.54 |
|--------------|--|------------------|----------------------------------|--------------------------|
| ATOM | 2444 O THR A 307 | 59.925 | | |
| ATOM | 2445 N LEU A 308 | 60.152 | | |
| MOTA | 2446 CA LEU A 308 | 60.172 | | |
| MOTA | 2447 CB LEU A 308 | 60.442 | | 1.00 19.20 |
| MOTA | 2448 CG LEU A 308 | 61.797 | 13.386 122.938 | |
| ATOM | 2449 CD1_LEU A 308 | 61.900 | 14.362 121.774 | |
| MOTA | 2450 CD2 LEU A 308 | 62.937 | | |
| ATOM | 2451 C LEU A 308 | 58.811 | | 1.00 25.18 |
| MOTA | 2452 O LEU A 308 | 58.731 | | |
| ATOM | 2453 N ILE A 309 | 57.743 | | |
| MOTA | 2454 CA . ILE A 309 | 56.394 | | |
| ATOM | 2455 CB ILE A 309 2456 CG2 ILE A 309 | 55.337 | | |
| MOTA | | 53.945 | 12.321 124.948 | |
| ATOM | 2457 CG1 ILE A 309 2458 CD1 ILE A 309 | 55.403 | | |
| ATOM ATOM | 2450 CDI ILE A 309 | 55.118 | | |
| ATOM | 2460 O ILE A 309 | 56.228 55.731 | | |
| ATOM | 2461 N TRP A 310 | 56.652 | | |
| ATOM | 2462 CA TRP A 310 | 56.525 | | |
| ATOM | 2463 CB TRP A 310 | 56.940 | 10.342 128.192 8.872 128.132 | |
| ATOM | 2464 CG TRP A 310 | 56.874 | 8.203 129.479 | |
| MOTA | 2465 CD2 TRP A 310 | 55.697 | 7.967 130.263 | 1.00 29.80 |
| ATOM- | 2466 CE2 TRP A 310 | 56.115 | 7.390 131.480 | 1.00 32.47 |
| ATOM | 2467 CE3 TRP A 310 | 54.329 | 8.189 130.055 | |
| MOTA | 2468 CD1 TRP A 310 | 57.926 | 7.770 130.232 | 1.00 33.42 |
| ATOM | 2469 NE1 TRP A 310 | 57.480 | 7.282 131.436 | 1.00 30.09 |
| MOTA | 2470 CZ2 TRP A 310 | 55.213 | 7.030 132.492 | 1.00 29.93 |
| ATOM | 2471 CZ3 TRP A 310 | 53.432 | 7.831 131.062 | 1.00 29.72 |
| ATOM | 2472 CH2 TRP A 310 | 53.881 | 7.259 132.265 | 1.00 24.53 |
| ATOM | 2473 C TRP A 310 | 57.308 | 11.048 129.293 | 1.00 33.49 |
| ATOM | 2474 O TRP A 310 2475 N CYS A 311 | 56.820 | 11.137 130.426 | 1.00 27.59 |
| ATOM ATOM | 2475 N CYS A 311 2476 CA CYS A 311 | 58.512 | 11.535 128.984 | 1.00 29.34 |
| ATOM | 2477 CB CYS A 311 | 59.305 60.722 | 12.247 129.994 | 1.00 30.06 |
| ATOM | 2478 SG CYS A 311 | 61.804 | 12.538 129.479 11.084 129.327 | 1.00 30.08 |
| ATOM | 2479 C CYS A 311 | 58.612 | 13.560 130.397 | 1.00 33.17 1.00 29.25 |
| ATOM | 2480 O CYS A 311 | 58.612 | 13.940 131.570 | 1.00 28.80 |
| ATOM | 2481 N GLU A 312 | 58.021 | 14.247 129.425 | 1.00 23.13 |
| ATOM | 2482 CA GLU A 312 | 57.308 | 15.496 129.696 | 1.00 30.31 |
| ATOM | 2483 CB GLU A 312 | 56.648 | 16.032 128.427 | 1.00 28.97 |
| MOTA | 2484 CG GLU A 312 | 57.080 | 17.418 127.988 | 1.00 41.67 |
| ATOM | 2485 CD GLU A 312 | 56.905 | 18.465 129.059 | 1.00 44.21 |
| ATOM | 2486 OE1 GLU A 312 | 55.813 | 18.534 129.658 | 1.00 54.15 |
| ATOM | 2487 OE2 GLU A 312 | 57.860 | 19.233 129.290 | 1.00 43.90 |
| MOTA | 2488 C GLU A 312 2489 O GLU A 312 | 56.204 | 15.225 130.712 | 1.00 28.03 |
| ATOM AOTA | 2489 O GLU A 312 2490 N LEU A 313 | 56.120 | 15.869 131.751 | 1.00 30.64 |
| ATOM | 2491 CA LEU A 313 | 55.343 54.231 | 14.270 130.388 | 1.00 31.06 |
| ATOM | 2492 CB LEU A 313 | 53.337 | 13.918 131.266 12.873 130.604 | 1.00 36.21 |
| ATOM | 2493 CG LEU A 313 | | 13.342 129.429 | 1.00 28.83 |
| ATOM | 2494 CD1 LEU A 313 | 51.818 | 12.146 128.788 | 1.00 34.62 1.00 33.05 |
| ATOM | 2495 CD2 LEU A 313 | 51.471 | 14.357 129.914 | 1.00 27.27 |
| ATOM | 2496 C LEU A 313 | 54.685 | 13.377 132.610 | 1.00 27.27 |
| MOTA | 2497 O LEU A 313 | 54.131 | 13.730 133.644 | 1.00 37.26 |
| MOTA | 2498 N SER A 314 | 55.688 | 12.508 132.577 | 1.00 33.72 |
| MOTA | 2499 CA SER A 314 | 56.233 | 11.880 133.776 | 1.00 33.58 |
| ATOM | 2500 CB SER A 314 | 57.183 | 10.743 133.388 | 1.00 35.88 |
| MOTA | 2501 OG SER A 314 | 56.517 | 9.761 132.628 | 1.00 45.88 |
| MOTA | 2502 C SER A 314 | 57.002 | 12.846 134.659 | 1.00 31.54 |
| MOTA | 2503 O SER A 314 | 57.339 | 12.513 135.788 | 1.00 27.69 |
| MOTA | 2504 N GLY A 315 | 57.312 | 14.021 134.130 | 1.00 35.50 |
| ATOM | 2505 CA GLY A 315 | 58.057 | 14.996 134.905 | 1.00 36.31 |
| MOTA | 2506 C GLY A 315 | | 14.634 135.099 | 1.00 38.47 |
| ATCM | 2507 O GLY A 315 | 60.138 | 15.049 136.078 | 1.00 41.57 |
| MOTA | 2508 N ARG A 316 | 60.089 | 13.862 134.181 | 1.00 39.32 |
| | | | | |

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| ATOM | 2509 CA ARG A 316 | 61.490 | 13.501 134.332 | 2 1 00 20 05 |
|------|----------------------|----------|----------------|--------------|
| MOTA | | 61.641 | 11.982 134.413 | |
| MOTA | | 61.233 | 11.226 133.184 | |
| ATOM | | 61.426 | 9.744 133.429 | |
| ATOM | 2513 NE ARG A 316 | | 9.744 133.429 | |
| ATOM | | 60.461 | | |
| ATOM | | 60.524 | | |
| | | 61.511 | | 1.00 38.93 |
| ATOM | 520 | 59.583 | | 1.00 30.53 |
| ATOM | 2517 C ARG A 316 | 62.369 | 14.083 133.230 | 1.00 40.17 |
| ATOM | 2518 O -ARG A 316 | 61.910 | 14.325 132.111 | 1.00 34.27 |
| MOTA | 2519 N GLU A 317 | 63.633 | | 1.00 41.26 |
| ATOM | 2520 CA GLU A 317 | 64.580 | 14.905 132.619 | 1.00 44.42 |
| AŤOM | 2521 CB GLU A 317 | 65.901 | 15.249 133.317 | 1.00 46.84 |
| ATOM | 2522 CG GLU A 317 | 65.756 | 15.996 134.629 | 1.00 40.84 |
| ATOM | 2523 CD GLU A 317 | 65.212 | 15.113 135.743 | |
| ATOM | 2524 OE1 GLU A 317 | 65.871 | 14 101 135.743 | |
| ATOM | 2525 OE2 GLU A 317 | | 14.101 136.073 | |
| MOTA | | 64.129 | 15.425 136.287 | |
| ATOM | | 64.873 | 13.962 131.462 | |
| | 2527 O GLU A 317 | 64.977 | 12.748 131.636 | |
| ATOM | 2528 N VAL A 318 | 65.010 | 14.525 130.275 | 1.00 37.64 |
| ATOM | 2529 CA VAL A 318 | 65.315 | 13.720 129.108 | 1.00 39.13 |
| ATOM | 2530 CB VAL A 318 | 64.858 | 14.417 127.810 | 1.00 42.75 |
| MOTA | 2531 CG1 VAL A 318 | 65.192 | 13.544 126.610 | 1.00 41.84 |
| ATOM | 2532 CG2 VAL A 316 | 63.364 | 14.701 127.867 | 1.00 42.38 |
| MOTA | 2533 C VAL A 318 | 66.822 | 13.495 129.037 | 1.00 38.45 |
| MOTA | 2534 O VAL A 318 | 67.598 | 14.442 128.910 | 1.00 38.45 |
| ATOM | 2535 N PRO A 319 | 67.261 | 12.236 129.156 | 1.00 36.04 |
| ATOM | 2536 CD PRO A 319 | 66.512 | 10 004 120 205 | 1.00 39.54 |
| ATOM | 2537 CA PRO A 319 | 68.695 | 10.994 129.397 | 1.00 40.47 |
| ATOM | 2538 CB PRO A 319 | . 68.745 | 11.949 129.088 | 1.00 43.85 |
| ATOM | 2539 CG PRO A 319 | | 10.439 129.319 | 1.00 44.12 |
| MOTA | | 67.419 | 9.986 128.745 | 1.00 46.48 |
| | | 69.228 | 12.353 127.718 | 1.00 43.55 |
| MOTA | 2541 O PRO A 319 | 68.563 | 12.141 126.708 | 1.00 43.45 |
| MOTA | 2542 N GLU A 320 | 70.420 | 12.936 127.689 | 1.00 42.52 |
| ATOM | 2543 CA GLU A 320 | 71.026 | 13.380 126.440 | 1.00 45.19 |
| MOTA | 2544 CB GLU A 320 | 72.384 | 14.032 126.706 | 1.00 43.86 |
| ATOM | 2545 CG GLU A 320 | 73.121 | 14.412 125.434 | 1.00 52.62 |
| ATOM | 2546 CD GLU A 320 | 74.507 | 14.967 125.697 | 1.00 52.36 |
| ATOM | 2547 OE1 GLU A 320 | 75.219 | 15.271 124.720 | 1.00 56.25 |
| ATOM | . 2548 OE2 GLU A 320 | 74.883 | 15.101 126.875 | 1.00 52.25 |
| ATOM | 2549 C GLU A 320 | 71.223 | 12.266 125.421 | 1.00 43.52 |
| ATOM | 2550 O GLU A 320 | 70.876 | 12.412 124.253 | 1.00 41.89 |
| ATOM | 2551 N LYS A 321 | 71.781 | 11.150 125.867 | 1.00 41.89 |
| ATOM | 2552 CA LYS A 321 | 72.059 | 10.041 124.969 | 1.00 43.35 |
| ATOM | 2553 CB LYS A 321 | 73.561 | 10.041 124.969 | 1.00 43.53 |
| ATOM | 2554 CG LYS A 321 | | 9.808 124.879 | 1.00 42.78 |
| ATOM | 2555 CD LYS A 321 | 74.238 | 9.34C 126.180 | 1.00 49.38 |
| ATOM | 2556 CE LYS A 321 | 74.272 | 10.396 127.307 | 1.00 57.82 |
| | | 72.978 | 10.497 128.129 | 1.00 53.81 |
| ATOM | 2557 NZ LYS A 321 | 72.660 | 9.245 128.883 | 1.00 54.17 |
| ATOM | 2558 C LYS A 321 | 71.407 | 8.731 125.345 | 1.00 41.52 |
| ATOM | 2559 O LYS A 321 | 70.954 | 8.540 126.469 | 1.00 41.98 |
| MOTA | 2560 N LEU A 322 | 71.378 | 7.820 124.382 | 1.00 38.64 |
| ATOM | 2561 CA LEU A 322 | 70.815 | 6.508 124.613 | 1.00 40.46 |
| MOTA | 2562 CB LEU A 322 | 70.442 | 5.845 123.289 | 1.00 42.22 |
| MOTA | 2563 CG LEU A 322 | 69.595 | 6.632 122.287 | 1.00 42.92 |
| ATOM | 2564 CD1 LEU A 322 | 69.204 | 5.737 121.125 | 1.00 42.92 |
| MOTA | 2565 CD2 LEU A 322 | 68.361 | | 1.00 41.13 |
| ATOM | 2566 C LEU A 322 | | 7.148 122.967 | 1.00 44.41 |
| | | 71.918 | 5.702 125.268 | 1.00 41.36 |
| ATOM | 2567 O LEU A 322 | 73.079 | 5.825 124.884 | 1.00 44.16 |
| MOTA | 2568 N ASN A 323 | 71.579 | 4.894 126.265 | 1.00 39.89 |
| MOTA | 2569 CA ASN A 323 | 72.594 | 4.067 126.895 | 1.00 40.96 |
| ATOM | 2570 CB ASN A 323 | 72.136 | 3.556 128.259 | 1.00 43.00 |
| ATOM | 2571 CG ASN A 323 | 70.787 | 2.886 128.202 | 1.00 45.59 |
| ATOM | 2572 OD1 ASN A 323 | 70.482 | 2.151 127.264 | 1.00 45.71 |
| ATOM | 2573 ND2 ASN A 323 | 69.975 | 3.114 129.224 | 1.00 48.08 |
| ATOM | 2574 C ASN A 323 | 72.828 | 2.894 125.954 | 1.00 44.88 |
| | | | ~.023 ~~00.003 | ~.UU **.00 |

| | ē. | |
|--------|-----------------------|--|
| AT | OM 2575 O ASN A 323 | 70 404 |
| AΤ | | 72.124 2.739 124.955 1.00 46.4 |
| | 11 329 | 73.809 2.062 126.268 1 00 45 0 |
| | 11514 A 324 | 74.122 0.938 125.404 1.00 49.8 |
| | - 15M A J24 | 75.386 0.244 125.904 1.00 53.8 |
| AT | | |
| AT | ODI ASN A 324 | 7. 2.4 |
| TA | DM 2581 ND2 ASN A 324 | |
| ATC | OM 2582 C ASN A 324 | 72 272 |
| ATC | OM 2583 O ASN A.324 | 70 704 |
| ATO | | /2./84 -U.644 124.197 1 00 43 67 |
| ATO | A 323 | 72.220 -0.276 126.339 1.00 46 30 |
| | 210 A 323 | 71.106 -1.221 126 318 1 00 46 76 |
| ATO | | 70.428 -1.328 127.695 1.00 47.65 |
| ATC | 215 A 323 | 7. 000 47.00 |
| ATC | | ======================================= |
| ATC | M 2589 CE LYS A 325 | 27 26.07 |
| ATC | M 2590 NZ LYS A 325 | 7, 000 37,43 |
| ATC | M 2591 C LYS A 325 | 70 36.32 |
| ATO | | 70.002 -0.791 125.296 1.00 45.17 |
| ATO | | 09.4/4 -1.625 124.601 1 00 42 72 |
| ATO | | 09.832 0.514 125.213 1.00 41 43 |
| | | 68.861 1.054 124 276 1 00 41 61 |
| ATO | | 68.562 2.508 124.616 1.00 42.80 |
| ATO: | | 50 55 20 20 20 20 20 20 20 20 20 20 20 20 20 |
| ATO | | |
| ATO! | M 2598 N LYS A 327 | |
| ATO | M 2599 CA LYS A 327 | 71 77 40 40 40 40 |
| ATO | M 2600 CB LYS A 327 | 70 700 43.26 |
| ATO | 1 2601 CG LYS A 327 | I.UU 44.// |
| ATOI | 1 2602 CD LYS A 327 | 7.00 30.07 |
| ATOM | 1 2603 CE LYS A 327 | 74.544 3.168 121.747 1.00 52.74 |
| ATOM | 1 2604 NZ LYS A 327 | 74.916 4.508 122.377 1.00 51 30 |
| ATOM | | 74.456 5.670 121.715 1 00 52 72 |
| ATOM | 220 7 327 | 71.063 -0.274 120 728 1 00 41 20 |
| | 11 327 | 70.625 -0.437 119.592 1 00 30 03 |
| ATOM | 11 520 | 71.403 -1.278 121.526 1.00 39.95 |
| ATOM | 71 520 | n |
| ATOM | 0-0 M 320 | |
| ATOM | 2610 CG GLU A 328 | 73 23 43.05 |
| ATOM | 2611 CD GLU A 328 | |
| ATOM | 2612 OE1 GLU A 328 | 7 |
| ATOM | 2613 OE2 GLU A 328 | 74 777 |
| ATOM | 2614 C GLU A 328 | 74.785 -2.558 120.584 1.00 51.64 |
| ATOM | 2615 O GLU A 328 | 69.825 -3.030 120.818 1.00 39.51 |
| ATOM | 2616 N LEU A 329 | 09.536 -3.842 119.939 1.00 37.35 |
| ATOM | | 68.911 -2.444 121.582 1.00 36.37 |
| ATOM | | 07.496 -2.717 121.380 1.00 36.03 |
| ATOM | | 66.646 -1,958 122,400 1,00 34 66 |
| | | 65.133 -2.110 122 213 1 00 22 00 |
| ATOM | 2620 CD1 LEU A 329 | 64.755 -3.572 122.351 1.00 36.21 |
| ATOM | 2621 CD2 LEU A 329 | 64.391 -1.268 123.240 1.00 34.00 |
| ATOM | 2622 C LEU A 329 | 67.120 -2.268 119.971 1.00 33.64 |
| · ATOM | 2623 O LEU A 329 | 7, |
| ATCM | 2624 N LEU A 330 | 50 31,29 |
| MOTA | 2625 CA LEU A 330 | 57 1.00 33.78 |
| ATOM | 2626 CB LEU A 330 | |
| MOTA | 2627 CG LEU A 330 | |
| ATOM | 2628 CD1 LEU A 330 | 66.514 1.958 119.205 1.00 31.51 |
| ATOM | 2629 CD2 LEU A 330 | 00.85/ 3.404 118.894 1.00 22 11 |
| ATOM | 220 2 330 | 05.028 1.728 118.978 1.00 29 69 |
| | | 9/./29 -1.201 117 246 1 00 36 40 |
| ATOM | 2631 O LEU A 330 | 67.142 -1.493 116.210 1 00 35 61 |
| ATOM | 2632 N LYS A 331 | 69.005 -1.503 117.455 1 00 27 62 |
| ATCM | 2633 CA LYS A 331 | 50 305 |
| ATOM | 2634 CB LYS A 331 | 71 0-2 |
| ATOM | 2635 CG LYS A 331 | 71 004 |
| ATOM | 2636 CD LYS A 331 | 77 77 2 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 |
| ATOM | 2637 CE LYS A 331 | 74 315 |
| ATOM | 2638 NZ LYS A 331 | 74.315 -1.889 116.765 1.00 53.71 |
| ATOM | | 73.928 -3.327 116.855 1.00 56.15 |
| ATOM | | 69.258 -3.612 116.173 1.00 42.35 |
| AI ON | 2640 O LYS A 331 | 69.310 -4.086 115.042 1.00 42.68 |
| | | |

| MOTA | 2641 | L N | SER A 3 | 332 | 68.734 | -4.270 | 117.200 | 1.00 | 41.56 |
|--------------|--------------|----------|------------------------|-----|------------------|----------------|------------------------|------|----------------|
| ATOM | 2642 | | SER A 3 | | 68.226 | -5.629 | | 1.00 | 46.88 |
| MOTA | 2643 | | SER A 3 | | 68.045 | -6.298 | | | 42.19 |
| ATOM | 2644 | | SER A 3 | | 66.959 | -5.71 | | | 39.55 |
| MOTA MOTA | 2645 2646 | | SER A 3 | | 66.896 66.393 | | 7 116.297 1 116.017 | | 48.58 |
| ATOM | 2647 | | ILE A 3 | | 66.325 | | 115.979 | | 45.78 48.27 |
| ATOM | 2648 | | ILE A 3 | | 65.041 | | 115.292 | | 51.82 |
| MOTA | 2649 | | ILE A 3 | | 64.378 | | 115.402 | | 52.16 |
| MOTA | 2650 | CG2 | | | 63.038 | | 114.683 | | 52.64 |
| ATOM | 2651 | | | | 64.163 | -2.765 | 116.871 | | 52.70 |
| ATOM | 2652 | | | | 63.550 | | 117.077 | | 56.70 |
| ATOM | 2653 | | ILE A 3 | | 65.112 | | 113.820 | | 53.43 |
| MOTA MOTA | 2654 2655 | N O | ILE A 3 ASP A 3 | | 66.118 64.016 | | 113.145 | | 56.45 |
| ATOM | 2656 | CA | ASP A 3 | | 63.865 | | 111.962 | | 55.53 59.58 |
| ATOM | 2657 | СВ | ASP A 3 | | 62.845 | | 111.918 | | 62.69 |
| ATOM | 2658 | CG | | 34 | 61.546 | | 112.664 | | 66.23 |
| ATOM | 2659 | OD1 | | 34 | 60.795 | -5.814 | 112.227 | | 63.25 |
| ATOM | 2660 | OD2 | | | 61.277 | | 113.704 | | 63.45 |
| ATOM | 2661 | C | ASP A 3 | | 63.385 | | 111.125 | | 60.81 |
| MOTA | 2662 2663 | O N | ASP A 3: PHE A 3: | | 62.239 64.266 | | 110.681 | | 59.47 |
| ATOM ATOM | 2664 | CA | PHE A 3 | | 63.864 | | 110.889 | | 60.00 59.37 |
| ATOM | 2665 | CB | PHE A 3 | | 64.247 | | 110.952 | 1.00 | 53.38 |
| ATOM | 2666 | CG | PHE A 33 | | 63.895 | -0.013 | 110.275 | 1.00 | 49.13 |
| MOTA | 2667 | CD1 | | | 62.618 | 0.189 | 109.770 | 1.00 | 44.32 |
| ATOM | 2668 | | PHE A 33 | | 64.845 | | 110.127 | | 49.91 |
| ATOM ATOM | 2669 2670 | CE1 | PHE A 33 | | 62.288 64.526 | 1.373 | 109.122 | | 42.74 |
| ATOM | 2671 | CZ | PHE A 33 | | 63.244 | | 109.403 | | 46.40 |
| ATOM | 2672 | c | PHE A 33 | | 64.334 | | 108.696 | | 60.85 |
| ATOM | 2673 | 0 | PHE A 33 | | 63.689 | | 107.785 | | 66.28 |
| ATOM | 2674 | N | GLU A 33 | | 65.430 | -1:671 | 108.493 | | 57.40 |
| ATOM | 2675 | CA | GLU A 33 | | 66.015 | | 107.174 | | 58.96 |
| ATOM | 2676 2677 | CB CG | GLU A 33 GLU A 33 | | 65.782 | | 106.211 | | 62.66 |
| MOTA MOTA | 2678 | CD | GLU A 33 | | 66.417 66.277 | -2.377 | 104.846 | | 68.51 73.21 |
| MOTA | 2679 | | GLU A 33 | | 66.753 | | 104.333 | | 73.30 |
| ATOM | 2680 | | GLU A 33 | | 65.697 | -3.457 | | | 75.74 |
| MOTA | 2681 | С | GLU A 33 | 6 | 65.460 | -0.124 | 106.576 | 1.00 | 55.70 |
| ATOM | 2682 | o | GLU A 33 | | 64.281 | -0.023 | | | 55.28 |
| ATOM | 2683 2684 | N | GLU A 33 | | 66.338 | 0.857 | | | 54.75 |
| ATOM ATOM | 2685 | CA CB | GLU A 33 | | 65.986 67.221 | 2.167 3.065 | | | 55.99 51.75 |
| ATOM | 2686 | CG | GLU A 33 | | 66.926 | | 106.092 | | 52.28 . |
| ATOM | 2687 | CD | GLU A 33 | | 66.184 | | 107.366 | | 43.72 |
| ATOM | 2688 | | GLU A 33 | | 66.705 | | 108.474 | | 42.21 |
| ATOM | 2689 | | GLU A 33 | | 65.072 | | 107.256 | | 47.31 |
| ATOM | 2690 | | GLU A 33' | | 65.485 | | 104.460 | | 57.56 |
| MOTA | 2691 2692 | | GLU A 33' PHE A 33' | | 66.087 64.385 | | 103.639 104.151 | 1.00 | |
| ATOM ATOM | 2693 | | PHE A 33 | | 63.814 | | 102.805 | 1.00 | |
| ATOM | 2694 | | PHE A 33 | | 62.561 | | 102.723 | 1.00 | |
| MOTA | 2695 | CG | PHE A 338 | 3 | 61.845 | | 101.401 | 1.00 | |
| ATOM | 2696 | | PHE A 338 | | 61.054 | | 101.094 | 1.00 | 62.99 |
| ATOM | 2697 | | PHE A 338 | | 61.970 | | 100.458 | 1.00 | |
| MOTA | 2698 | | PHE A 338 PHE A 338 | | 60.392 | 2.302 | 99.868 | 1.00 | |
| MOTA | 2699 2700 | | PHE A 338 | | 61.315 60.523 | 4.428 | 99.228 98.934 | 1.00 | |
| ATOM ATOM | 2701 | | PHE A 338 | | 64.818 | 3.208 | 101.773 | 1.00 | |
| ATOM | 2702 | | PHE A 338 | | 64.803 | | 100.616 | 1.00 | |
| ATOM | 2703 | - | ASP A 339 | | 65.677 | 4.130 | 102.194 | 1.00 | |
| ATOM · | 2704 | - | ASP A 339 | | 66.689 | | 101.310 | 1.00 | |
| ATCM | 2705 | | ASP A 339 | | 66.565 | | 101.248 | 1.00 | _ |
| ATCM | 2706 | CG A | ASP A 339 | • | 67.647 | 6.838 | 100.402 | 1.00 | P8.U3 |

| MOTA | 2707 OD1 ASP A 339 | 67.796 | 6.432 99.229 | 1 00 72 20 |
|-------|--------------------|--------|-----------------------------|------------|
| ATOM | | 68.346 | | |
| ATOM | | | | |
| ATOM | | 68.088 | | |
| | | 68.511 | | |
| ATOM | | 68.796 | | 1.00 71.90 |
| MOTA | | 70.151 | 3 ⁻ .111 101.149 | 1.00 73.59 |
| ATOM | 2713 CB ASP A 340 | 70,778 | 2.601 99.848 | 1.00 75.47 |
| MOTA | 2714 CG ASP A 340 | 69.953 | 1.511 99.195 | |
| MOTA | 2715 OD1 ASP A 340 | 69.761 | | |
| ATOM | | 69.492 | | |
| ATOM | 2717 C ASP A 340 | | 1.718 98.054 | |
| | | 71.069 | 4.155 101.766 | |
| ATOM | 2718 O ASP A 340 | 71.618 | 3.946 102.845 | 1.00 73.08 |
| MOTA | 2719 N GLU A 341 | 71.242 | 5.275 101.074 | 1.00 73.15 |
| ATOM | 2720 CA GLU A 341 | 72.112 | 6.341 101.557 | 1.00 74.56 |
| ATOM | 2721 CB GLU A 341 | 72.917 | 6.924 100.390 | 1.00 77.06 |
| MOTA | 2722 CG GLU A 341 | 73.878 | 8.034 100.792 | 1.00 //.06 |
| ATOM | 2723 CD GLU A 341 | 74.924 | 3.034 100.792 | |
| ATOM | 2724 071 077 - 244 | | 7.571 101.794 | 1.00 85.34 |
| | | | 6.669 101.450 | 1.00 86.64 |
| MOTA | | 74.951 | 8.106 102.924 | 1.00 85.37 |
| ATOM | 2726 C GLU A 341 | 71.327 | 7.453 102.245 | 1.00 72.47 |
| MOTA | . 2727 O GLU A 341 | 70.822 | 8.364 101.589 | 1.00 76.75 |
| MOTA | 2728 N VAL A 342 | 71.228 | 7.381 103.566 | 1.00 67.86 |
| MOTA | 2729 CA VAL A 342 | 70.503 | 8.393 104.323 | 1.00 64.84 |
| ATOM | 2730 CB VAL A 342 | 69.160 | | 1.00 64.84 |
| ATOM | 2731 CG1 VAL A 342 | 68.256 | | 1.00 66.27 |
| MOTA | 2732 CG2 VAL A 342 | | 7.494 103.701 | 1.00 67.95 |
| ATOM | 2733 C VAL A 342 | 69.400 | 6.637 105.722 | 1.00 65.37 |
| | | 71.305 | 8.871 105.520 | 1.00 61.75 |
| MOTA | | 71.375 | 10.066 105.795 | 1.00 64.14 |
| ATOM | 2735 N ASP A 343 | 71.912 | 7.925 106.225 | 1.00 56.79 |
| ATOM- | 2736 CA ASP A 343 | 72.692 | 8.229 107.417 | 1.00 54.53 |
| ATOM | 2737 CB ASP A 343 | 73.707 | 9.340 107.158 | 1.00 56.31 |
| ATOM | 2738 CG ASP A 343 | 74.531 | 9.660 108.388 | 1.00 58.81 |
| ATOM | 2739 OD1 ASP A 343 | 75.298 | 10.644 108.357 | |
| ATOM | 2740 OD2 ASP A 343 | 74.420 | | 1.00 65.36 |
| ATOM | 2741 C ASP A 343 | | 8.918 109.387 | 1.00 54.29 |
| ATOM | 2742 O ASP A 343 | 71.765 | 8.675 108.534 | 1.00 50.70 |
| | 2743 N ARG A 344 | 71.442 | 9.859 108.651 | 1.00 46.00 |
| MOTA | | 71.328 | 7.717 109.341 | 1.00 46.20 |
| ATOM | 2744 CA ARG A 344 | 70.452 | 8.004 110.463 | 1.00 41.18 |
| MOTA | 2745 CB ARG A 344 | 69.121 | 7.268 110.299 | 1.00 39.81 |
| ATOM | 2746 CG ARG A 344 | 68.289 | 7.711 109.098 | 1.00 35.08 |
| ATOM | 2747 CD ARG A 344 | 68.036 | 9.211 109.121 | 1.00 28.37 |
| ATOM | 2748 NE ARG A 344 | 67.157 | 9.645 108.036 | 1.00 30.90 |
| ATOM | 2749 CZ ARG A 344 | 67.013 | 10.909 107.649 | 1.00 30.90 |
| ATOM | 2750 NH1 ARG A 344 | 67.693 | | 1.00 31.05 |
| ATOM | 2751 NH2 ARG A 344 | | | 1.00 30.49 |
| ATOM | 2752 C ARG A 344 | 66.201 | 11.212 106.646 | 1.00 31.76 |
| | | 71.147 | 7.561 111,742 | 1.00 38.46 |
| ATOM | | 70.516 | 7.370 112.773 | 1.00 34.99 |
| MOTA | 2754 N SER A 345 | 72.464 | 7.418 111.662 | 1.00 33.97 |
| MOTA | 2755 CA SER A 345 | 73.261 | 6.981 112.795 | 1.00 33.68 |
| ATOM | 2756 CB SER A 345 | 74.742 | 6.972 112.404 | 1.00 39.11 |
| MOTA | 2757 OG SER A 345 | 75.163 | 8.260 111.990 | 1.00 42.80 |
| ATOM | 2758 C SER A 345 | 73.054 | 7.826 114.053 | 1.00 31.83 |
| ATOM | 2759 O SER A 345 | 73.100 | 7.314 115.167 | 1.00 31.83 |
| ATOM | 2760 N TYR A 346 | 72.819 | 9.119 113.877 | 1.00 24.35 |
| | 2761 CA TYR A 346 | | 9.119 113.8// | 1.00 33.10 |
| ATOM | | | 10.003 115.015 | 1.00 34.50 |
| ATOM | 2762 CB TYR A 346 | | 11.437 114.522 | 1.00 35.16 |
| ATOM | 2763 CG TYR A 346 | | 11.615 113.659 | 1.00 39.69 |
| ATOM | 2764 CD1 TYR A 346 | 69.909 | 11.814 114.227 | 1.00 36.57 |
| ATOM | 2765 CE1 TYR A 346 | 68.767 | 11.940 113.424 | 1.00 40.23 |
| ATOM | 2766 CD2 TYR A 346 | 71.260 | | 1.00 39.04 |
| ATOM | 2767 CE2 TYR A 346 | | | 1 00 30 65 |
| ATOM | 2768 CZ TYR A 346 | | | 1.00 38.65 |
| | 2769 OH TYR A 346 | | | 1.00 37.64 |
| MOTA | | | 11.982 111.234 | 1.00 32.48 |
| ATOM | | 71.432 | 9.560 115.874 | 1.00 37.72 |
| ATCM | 2771 O TYR A 346. | 71.396 | 9.829 117.074 | 1.00 35.48 |
| ATCM | 2772 N MET A 347 | 70.472 | 8.869 115.265 | 1.00 35.36 |
| | | | | |

| ATOM | 2773 CA MET A 347 | 69.295 | 8.418 116.004 | 1.00 36.97 |
|--------------|--|------------------|----------------------------------|--------------------------|
| MOTA | 2774 CB MET A 347 | 68.226 | 7.868 115.052 | |
| MOTA | 2775 CG MET A 347 | 67.853 | | |
| MOTA MOTA | 2776 SD MET A 347 2777 CE MET A 347 | 66.471 | | |
| ATOM- | 2778 C MET A 347 | 67.058 69.632 | | |
| ATOM | 2779 O MET A 347 | 68.890 | | |
| MOTA | 2780 N LEU A 348 | 70.747 | | |
| ATOM | 2781 CA LEU A 348 | 71.137 | 5.641 117.846 | 1.00 34.57 |
| MOTA | 2782 CB -LEU A 348 | 71.841 | | 1.00 34.16 |
| MOTA MOTA | 2783 CG LEU A 348 2784 CD1 LEU A 348 | 71.066 72.010 | | 1.00 35.61 |
| MOTA | 2785 CD2 LEU A 348 | 69.906 | 2.660 115.469 2.935 116.788 | 1.00 36.58 |
| MOTA | 2786 C LEU A 348 | 72.075 | 6.232 118.885 | 1.00 42.34 1.00 37.10 |
| MOTA | 2787 O LEU A 348 | 72.583 | 5.513 119.745 | 1.00 37.75 |
| MOTA | 2788 N GLU A 349 | 72.295 | 7.541 118.801 | 1.00 38.31 |
| MOTA | 2789 CA GLU A 349 2790 CB GLU A 349 | . 73.192 | 8.231 119.726 | 1.00 42.86 |
| MOTA MOTA | 2790 CB GLU A 349 . 2791 CG GLU A 349 | 74.150 74.942 | 9.136 118.948 8.426 117.867 | 1.00 47.04 |
| ATOM | 2792 CD GLU A 349 | 75.828 | 8.426 117.867 7.325 118.410 | 1.00 53.27 1.00 58.36 |
| MOTA | 2793 OE1 GLU A 349 | 76.681 | 7.619 119.279 | 1.00 59.59 |
| MOTA | 2794 OE2 GLU A 349 | 75.669 | 6.166 117.963 | 1.00 59.17 |
| ATOM | 2795 C GLU A 349 | 72.458 | 9.080 120.752 | 1.00 41.72 |
| ATOM ATOM | 2796 O GLU A 349 2797 N THR A 350 | 72.564 | | 1.00 42.27 |
| ATOM | 2798 CA THR A 350 | 71.716 70.992 | 10.067 120.261 10.976 121.135 | 1.00 37.05 1.00 40.78 |
| MOTA | 2799 CB THR A 350 | 71.468 | 12.418 120.900 | 1.00 40.78 |
| MOTA | 2800 OG1 THR A 350 | 71.359 | 12.733 119.508 | 1.00 43.25 |
| MOTA | 2801 CG2 THR A 350 | 72.918 | 12.575 121.325 | 1.00 44.11 |
| ATOM ATOM | 2802 C THR A 350 2803 O THR A 350 | . 69.474 | 10.911 120.968 | 1.00 41.47 |
| ATOM | 2804 N LEU A 351 | 68.968 68.760 | 10.608 119.884 11.199 122.054 | 1.00 39.72 1.00 38.68 |
| ATOM | 2805 CA LEU A 351 | 67.299 | 11.185 122.056 | 1.00 35.91 |
| MOTA | 2806 CB LEU A 351 | 66.763 | 11.210 123.487 | 1.00 35.94 |
| MOTA | 2807 CG LEU A 351 | 66.752 | 9.890 124.251 | 1.00 37.67 |
| MOTA MOTA | 2808 CD1 LEU A 351 2809 CD2 LEU A 351 | 66.290 65.813 | 10.118 125.677 8.920 123.544 | 1.00 40.11 |
| ATOM | 2810 C LEU A 351 | 66.679 | 8.920 123.544 12.342 121.294 | 1.00 39.29 1.00 37.76 |
| ATOM | 2811 O LEU A 351 | 65.747 | 12.149 120.512 | 1.00 34.86 |
| ATOM | 2812 N LYS A 352 | 67.192 | 13.544 121.525 | 1.00 34.79 |
| ATOM | 2813 CA LYS A 352 2814 CB LYS A 352 | 66.651 | 14.724 120.870 | 1.00 38.73 |
| MOTA MOTA | 2814 CB LYS A 352 2815 CG LYS A 352 | 66.676 66.062 | 15.911 121.835 15.580 123.179 | 1.00 36.48 |
| ATOM | 2816 CD LYS A 352 | 66.202 | 16.701 124.196 | 1.00 42.08 1.00 43.22 |
| ATOM | 2817 CE LYS A 352 | 65.349 | 17.901 123.845 | 1.00 49.81 |
| ATOM | 2818 NZ LYS A 352 | 65.342 | 18.880 124.972 | 1.00 52.70 |
| ATOM | 2819 C LYS A 352 2820 O LYS A 352 | 67.425 | 15.063 119.610 | 1.00 38.77 |
| ATOM ATOM | 2820 O LYS A 352 2821 N ASP A 353 | 68.654 66.697 | 15.098 119.601 15.293 118.530 | 1.00 36.21 |
| ATOM | 2822 CA ASP A 353 | 67.337 | 15.647 117.286 | 1.00 37.69 1.00 39.89 |
| ATOM | 2823 CB ASP A 353 | 66.532 | 15.075 116.110 | 1.00 43.53 |
| MOTA | 2824 CG ASP A 353 | 65.058 | 15.368 116.211 | 1.00 47.99 |
| ATOM | 2825 OD1 ASP A 353 | 64.253 | 14.623 115.593 | 1.00 38.06 |
| ATOM | 2826 OD2 ASP A 353 2827 C ASP A 353 | 64.706 67.457 | 16.352 116.898 | 1.00 52.94 |
| ATOM ATOM | 2828 O ASP A 353 | 66.890 | 17.165 117.247 17.861 118.092 | 1.00 39.20 1.00 35.66 |
| ATOM | 2829 N PRO A 354 | 68.244 | 17.696 116.302 | 1.00 40.75 |
| ATOM | 2830 CD PRO A 354 | 69.047 | 17.005 115.279 | 1.00 40.05 |
| ATOM | 2831 CA PRO A 354 | 68.426 | 19.145 116.179 | 1.00 38.41 |
| ATOM | 2832 CB PRO A 354 2833 CG PRO A 354 | 69.534 | 19.250 115.140 | 1.00 36.24 |
| MOTA MOTA | 2833 CG PRO A 354 2834 C PRO A 354 | 69.190 67.144 | 18.095 114.225 19.780 115.689 | 1.00 39.41 |
| ATOM | 2835 O PRO A 354 | 66.299 | 19.106 115.094 | 1.00 37.28 |
| ATOM | 2836 N TRP A 355 | 66.993 | 21.074 115.934 | 1.00 37.87 |
| MOTA | 2837 CA TRP A 355 | 65.804 | 21.757 115.472 | 1.00 40.04 |
| atom | 2838 CB TRP A 355 | 65.714 | 23.157 116.080 | 1.00 42.85 |

| | | | • | | |
|--------------|--------------|------------------------------|------------------|----------------------------------|--------------------------|
| ATOM | 2839 | G TRP A 355 | 64.333 | 3 23.471 116.569 | 1.00 53.01 |
| ATOM | 2840 | CD2 TRP A 355 | 63.439 | | |
| MOTA | 2841 | L CE2 TRP A 355 | 62.234 | 24.368 116.783 | |
| MOTA | 2842 | | 63.538 | 25.422 115.028 | |
| MOTA | | | 63.655 | 22.836 117.575 | |
| MOTA | 2844 | | 62.393 | | |
| ATOM | 2845 | | 61.134 | 25.197 116.532 | 1.00 51.28 |
| MOTA | 2846 | | 62.444 | | 1.00 53.22 |
| ATOM | 2847 | | 61.257 | | 1.00 50.50 |
| MOTA | 2848 | | 65.935 | | 1.00 37.34 |
| ATOM | 2849 | | 67.041 | | 1.00 39.01 |
| ATOM | 2850 | | 64.809 | | 1.00 36.31 |
| ATOM | 2851 2852 | | 64.797 | - | 1.00 35.22 |
| MOTA | | | | | 1.00 33.36 |
| MOTA | 2853 2854 | CG ARG A 356 CD ARG A 356 | 65.310 | _ | 1.00 34.50 |
| ATOM | 2855 | NE ARG A 356 | 64.729 65.745 | 17.927 111.468 16.956 111.870 | 1.00 28.06 |
| MOTA MOTA | 2856 | CZ ARG A 356 | 65.499 | 15.703 112.236 | 1.00 24.79 |
| MOTA | 2857 | NH1 ARG A 356 | 64.253 | 15.237 112.259 | 1.00 27.56 1.00 19.09 |
| ATOM | 2858 | NH2 ARG A 356 | 66.502 | 14.918 112.604 | 1.00 19.09 |
| ATOM | 2859 | C ARG A 356 | 63.874 | 22.955 111.390 | 1.00 21.34 |
| ATOM | 2860 | O ARG A 356 | 62.746 | 22.732 110.950 | 1.00 34.68 |
| MOTA | 2861 | N GLY A 357 | 64.361 | 24.181 111.550 | 1.00 35.60 |
| ATOM | 2862 | CA GLY A 357 | 63.556 | 25.345 111.220 | 1.00 35.43 |
| MOTA | 2863 | C GLY A 357 | 63.719 | 25.932 109.830 | 1.00 38.08 |
| MOTA | 2864 | O GLY A 357 | 64.112 | 25.250 108.885 | 1.00 37.29 |
| ATOM | 2865 | N GLY A 358 | 63.406 | 27.218 109.721 | 1.00 39.67 |
| MOTA | 2866 | CA GLY A 358 | 63.493 | 27.925 108.457 | 1.00 36.36 |
| MOTA | 2867 | C GLY A 358 | 62.398 | 28.966 108.499 | 1.00 39.45 |
| MOTA | 2868 | O GLY A 358 | 61.763 | 29.131 109.539 | 1.00 37.58 |
| ATOM | 2869 2870 | N GLU A 359 CA GLU A 359 | 62.163 | 29.662 107.391 | 1.00 40.89 |
| ATOM ATOM | 2871 | CA GLU A 359 CB GLU A 359 | 61.121 | 30.682 107.358 31.627 106.172 | 1.00 41.37 |
| ATOM | 2872 | CG GLU A 359 | 61.310 60.956 | 31.627 106.172 30.977 104.848 | 1.00 44.64 |
| ATOM | . 2873 | CD GLU A 359 | 60.833 | 31.973 103.708 | 1.00 52.13 1.00 59.14 |
| MOTA | 2874 | OE1 GLU A 359 | 60.448 | 31.551 102.593 | 1.00 59.14 |
| ATOM | 2875 | OE2 GLU A 359 | 61.119 | 33.173 103.923 | 1.00 57.77 |
| MOTA | 2876 | C GLU A 359 | 59.770 | 30.006 107.200 | 1.00 38.02 |
| ATOM | 2877 | O GLU A 359 | 59.689 | 28.828 106.850 | 1.00 35.29 |
| ATOM | . 2878 | N VAL A 360 | 58.708 | 30.762 107.441 | 1.00 36.81 |
| MOTA | 2879 | CA VAL A 360 | 57.363 | 30.237 107.291 | 1.00 35.97 |
| ATOM | 2880 | CB VAL A 360 | 56.401 | 30.789 108.368 | 1.00 34.90 |
| ATOM | 2881 | CG1 VAL A 360 | 54.999 | 30.251 108.133 | 1.00 36.53 |
| ATOM | 2882 | CG2 VAL A 360 | 56.888 | 30.393 109.755 | 1.00 37.06 |
| MOTA | 2883 | C VAL A 360 | 56.886 | 30.690 105.928 | 1.00 36.74 |
| ATOM | 2884 | O VAL A 360 | 56.661 | 31.881 105.712 | 1.00 34.90 |
| ATOM | 2885 2886 | N ARG A 361 CA ARG A 361 | 56.753 56.301 | 29.741 105.004 | 1.00 35.48 |
| ATOM | 2887 | CB ARG A 361 | 56.152 | 30.049 103.652 28.776 102.815 | 1.00 38.21 1.00 39.76 |
| ATOM ATOM | 2888 | CG ARG A 361 | 57.416 | 28.342 102.098 | 1.00 39.76 |
| ATOM | 2889 | CD ARG A 361 | 57.225 | | |
| ATCM | 2890 | NE ARG A 361 | 57.112 | 25.940 102.525 | 1.00 39.72 |
| ATOM | 2891 | CZ ARG A 361 | 56.952 | 24.643 102.286 | 1.00 38.79 |
| ATOM | 2892 | NH1 ARG A 361 | 56.881 | 24.200 101.036 | 1.00 32.40 |
| MOTA | 2893 | NH2 ARG A 361 | 56.899 | 23.785 103.297 | 1.00 36.58 |
| ATOM | 2894 | C ARG A 361 | 54.996 | 30.807 103.603 | 1.00 38.98 |
| ATOM | 2895 | O ARG A 361 | 54.120 | 30.636 104.452 | 1.00 39.07 |
| ATCM | 2896 | N LYS A 362 | 54.880 | 31.634 102.573 | 1.00 39.95 |
| MOTA | 2897 | CA LYS A 362 | 53.709 | 32.459 102.339 | 1.00 42.73 |
| ATCM | 2898 | CB LYS A 362 | 53.931 | 33.301 101.078 | 1.00 44.92 |
| atch : | 2899 | CG LYS A 362 | 54.995 | 34.390 101.219 | 1.00 55.45 |
| ATCM | 2900 | CD LYS A 362 | 56.351 | 33.842 101.671 | 1.00 58.28 |
| ATCM | 2901 | CE LYS A 362 | 56.907 | 32.809 100.697 | 1.00 57.34 |
| ATOM | _ | NZ LYS A 362 | 58.224 | 32.283 101.151 | 1.00 58.75 |
| ATOM | | C LYS A 362 | 52.434 | 31.634 102.200 | 1.00 40.51 |
| ATCM | 2904 | O LYS A 362 | 51.391 | 31.996 102.748 | 1.00 36.10 |

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Figure 18-45

| | • | |
|--------------|--|--|
| ATC | | 52.506 30.527 101.469 1.00 37.79 |
| ATO | M 2906 CA GLU A 363 | 51.313 29.705 101.295 1 00 40 96 |
| ATO | | 51.587 28.530 100.347 1.00 43.62 |
| ATO ATO | 11 303 | 52.729 27.616 100.739 1.00 47 01 |
| ATO | | 52.995 26.547 99.683 1.00 51.65 |
| ATO: | | 52.080 25.737 99.409 1.00 45.63 |
| ATO | 0-0 11 303 | 54.116 26.526 99.125 1.00 48.44 50.788 29.209 102.636 1.00 37.74 |
| ATO | | 1 |
| ATO | M 2914 N VAL A 364 | 1.00 34.79 |
| ATO | M 2915 CA VAL A 364 | 51.691 28.910 103.564 1.00 33.64 51.274 28.455 104.886 1.00 32.39 |
| ATO | | 52.484 28.048 105.749 1.00 33.99 |
| ATO | | 52.018 27.676 107.160 1.00 36.90 |
| OTA ATO | 501 | 53.198 26.867 105.109 1.00 29.56 |
| ATOM | | 50.506 29.574 105.589 1.00 34.33 |
| ATON | 1 2921 N LYS A 365 | 49.454 29.336 106.188 1.00 29.80 51.027 30.797 105.499 1.00 38.13 |
| ATON | 1 2922 CA LYS A 365 | 2.00 30.12 |
| ATOM | 2923 CB LYS A 365 | |
| ATOM | 1 2924 CG LYS A 365 | 51.255 33.204 105.969 1.00 37.98 52.629 33.084 106.610 1.00 37.99 |
| ATOM | 505 | 53.449 34.357 106.429 1.00 35 50 |
| ATOM | | 54.837 34.190 107.032 1.00 40.35 |
| ATOM ATOM | | 55.674 35.407 106.877 1.00 43.74 |
| ATOM | 2929 O LYS A 365 | 49.025 32.191 105.468 1.00 36.62 |
| ATOM | | 48.038 32.469 106.148 1.00 33.53 48.968 32.073 104.147 1.00 37.05 |
| ATOM | 2931 CA ASP A 366 | 48.968 32.073 104.147 1.00 37.05 47.708 32.278 103.449 1.00 37.72 |
| ATOM | 2932 CB ASP A 366 | 47.906 32.237 101.929 1.00 40.57 |
| ATOM | | 48.833 33.334 101.427 1.00 43 98 |
| MOTA MOTA | 2934 OD1 ASP A 366 2935 OD2 ASP A 366 | 49.078 34.304 102.176 1.00 38.51 |
| ATOM | 2936 C ASP A 366 | 49.297 33.235 100.269 1.00 41.96 |
| ATOM | 2937 O ASP A 366 | 46.670 31.238 103.862 1.00 39.24 45.497 31.562 104.029 1.00 39.04 |
| ATOM | 2938 N THR A 367 | |
| ATOM | 2939 CA THR A 367 | 47.096 29.990 104.031 1.00 38.99 46.167 28.935 104.432 1.00 36.80 |
| ATOM | 2940 CB THR A 367 | 46.868 27.560 104.527 1.00 33.84 |
| ATOM ATOM | 2941 OG1 THR A 367 2942 CG2 THR A 367 | 47.332 27.167 103.232 1.00 34.92 |
| ATOM | 2942 CG2 THR A 367 2943 C THR A 367 | 45.904 26.509 105.046 1.00 35.11 |
| АТОЙ | 2944 O THR A 367 | 45.532 29.257 105.786 1.00 36.58 44.307 29.202 105.931 1.00 30 18 |
| ATOM | 2945 N LEU A 368 | |
| MOTA | 2946 CA LEU A 368 | 46.363 29.581 106.776 1.00 35.32 45.850 29.926 108.095 1.00 35.46 |
| MOTA | 2947 CB LEU A 368 | 46.997 30.169 109.077 1.00 34.03 |
| ATOM | 2948 CG LEU A 368 | 47.545 28.925 109.794 1.00 39.04 |
| MOTA MOTA | 2949 CD1 LEU A 368 2950 CD2 LEU A 368 | 46.449 28.358 110.688 1.00 37.35 |
| ATOM | 2951 C LEU A 368 | 48.014 27.871 108.797 1.00 39.52 |
| ATOM | 2952 O LEU A 368 | 44.957 31.156 107.994 1.00 38.12 43.968 31.277 108.719 1.00 31.70 |
| ATOM | 2953 N GLUA 369 | 43.968 31.277 108.719 1.00 31.70 45.307 32.063 107.086 1.00 40.45 |
| ATOM | 2954 CA GLU A 369 | 44.509 33.261 106.866 1.00 45.36 |
| ATOM | 2955 CB GLU A 369 | 45.128 34.126 105.765 1.00 47.38 |
| ATOM | 2956 CG GLU A 369 | 46.020 35.228 106.283 1.00 53.81 |
| MOTA MOTA | 2957 CD GLU A 369 2958 OE1 GLU A 369 | 45.227 36.306 106.996 1.00 59.97 |
| ATOM | 2959 OE2 GLU A 369 | 45.846 37.252 107.526 1.00 60.65 |
| ATOM | 2960 C GLU A 369 | 43.980 36.211 107.016 1.00 63.69 43.100 32.865 106.466 1.00 43.33 |
| ATOM | 2961 O GLU A 369 | 2.00 43.23 |
| MOTA | 2962 N LYS A 370 | 42.130 33.283 107.095 1.00 44.62 42.983 32.057 105.417 1.00 40.34 |
| MOTA | 2963 CA LYS A 370 | 41.666 31.631 104.977 1.00 43.36 |
| ATOM | 2964 CB LYS A 370 | 41.738 30.773 103.704 1.00 44.79 |
| ATOM | 2965 CG LYS A 370 | 42.032 31.546 102.419 1.00 48.93 |
| ATOM | 2966 CD LYS A 370 2967 CE LYS A 370 | 43.503 31.514 102.019 1.00 51.41 |
| ATOM ATOM | 2968 NZ LYS A 370 | 43.921 30.116 101.561 1.00 51.14 45.339 30.062 101.091 1.00 50.34 |
| ATOM | 2969 C LYS A 370 | 40 050 |
| ATOM | 2970 O LYS A 370 | 20 745 |
| | - | 39.745 30.977 106.248 1.00 41.34 |

| ATOM | 2971 N ALA | 371 | 41.715 | 30 035 | 106.802 | 2 1 00 20 55 |
|--------------|---------------------------------|----------|------------------|----------------|------------------|--------------------------|
| ATOM | | | 41.120 | | 100.802 | |
| ATOM | # · · · | | 42.193 | | 107.86. | |
| ATOM | | | 40.365 | 30.132 | | |
| ATOM | | | 39.230 | 29.829 | | |
| ATOM | 2976 N LYS A | | 40.981 | | 109.210 | |
| MOTA | 2977 CA LYS A | | 40.391 | 32.178 | | |
| ATOM | 2978 C LYS A | 372 | 39.052 | 32.178 | | |
| ATOM | 2979 O LYS A | | 38.294 | 33.318 | | |
| ATOM | 2980 CB LYS A | | 41.334 | 33.364 | | |
| MOTA | 2981 CG LYS A | | 42.804 | 32.949 | | |
| ATOM | 2982 CD LYS A | | 43.746 | 34.131 | | |
| MOTA | 2983 CE LYS A | | 45.216 | 33.715 | | |
| ATOM | 2984 NZ LYS A | | 46.121 | 34.850 | | |
| ATOM | 2985 N ALA A | | 38.751 | 32.476 | | |
| ATOM | 2986 CA ALA A | | 37.492 | 32.933 | 107.806 | |
| MOTA | 2987 CB ALA A | | 37.758 | 33.632 | 106.480 | |
| MOTA | 2988 C ALA A | | 36.524 | 31.773 | 107.594 | |
| ATOM | 2989 O ALA A | 373 | 35.432 | 31.797 | 108.205 | 1.00 59.58 |
| ATOM | 2990. OXT ALA A | 373 | 36.870 | 30.853 | 106.822 | 1.00 60.10 |
| MOTA | 3014 CB ALA B | 2 | 54.881 | -4.431 | 56.836 | 1.00 55.77 |
| MOTA | 3015 C ALA B | 2 | 53.960 | -2.137 | 56.480 | 1.00 57.58 |
| MOTA | 3016 O ALA B | 2 | 54.920 | -1.720 | 57.131 | 1.00 56.75 |
| MOTA | 3017 N ALA B | 2 | 54.263 | -3.672 | 54.557 | 1.00 58.22 |
| MOTA | 3018 CA ALA B | 2 | 53.914 | -3.584 | 56.008 | 1.00 58.47 |
| MOTA | 3019 N LYS B | 3 | 52.919 | -1.376 | 56.151 | 1.00 52.79 |
| ATOM | 3020 CA LYS B | 3 | 52.855 | 0.022 | 56.543 | 1.00 49.68 |
| MOTA | 3021 CB LYS B | 3 | 51.643 | 0.700 | 55.896 | 1.00 53.14 |
| ATOM | 3022 CG LYS B | 3 | 51.751 | 0.785 | 54.377 | 1.00 53.37 |
| ATOM | 3023 CD LYS B | 3 | 50.685 | 1.681 | 53.786 | 1.00 55.40 |
| ATOM | 3024 CE LYS B | 3 | 50.808 | 1.783 | 52.277 | 1.00 59.51 |
| MOTA | 3025 NZ LYS B | 3 | 52.140 | 2.323 | 51.884 | 1.00 56.88 |
| MOTA | 3026 C LYS B 3027 O LYS B | 3 | 52.849 | 0.238 | 58.059 | 1.00 46.83 |
| ATOM ATOM | 3027 O LYS B 3028 N VAL B | 3. | 52.389 | -0.607 | 58.830 | 1.00 41.63 |
| ATOM | 3029 CA VAL B | · 4 4 | 53.376 | 1.385 | 58.467 | 1.00 41.46 |
| ATOM | 3030 CE VAL B | 4 | 53.483 | 1.751 | 59.871 | 1.00 40.85 |
| ATOM | 3031 CG1 VAL B | 4 | 54.893 55.070 | 2.288 | 60.163 | 1.00 39.55 |
| ATOM | 3032 CG2 VAL B | 4 | 55.916 | 2.541 1.306 | 61.648 59.652 | 1.00 41.23 |
| ATOM | 3033 C VAL B | 4 | 52.451 | 2.813 | 60.230 | 1.00 38.96 |
| ATOM | 3034 O VAL B | 4 | 52.472 | 3.916 | 59.691 | 1.00 38.92 1.00 42.80 |
| ATOM | 3035 N LYS B | 5 | 51.559 | 2.479 | 61.157 | 1.00 34.90 |
| MOTA | 3036 CA LYS B | 5 | 50.501 | 3.396 | 61.558 | 1.00 31.22 |
| MOTA | 3037 CE LYS B | 5 | 49.133 | 2.796 | 61.215 | 1.00 33.76 |
| ATOM | 3038 CG LYS B | 5 | 48.841 | 2.623 | 59.726 | 1.00 36.60 |
| ATOM | 3039 CD LYS B | 5 | 48.667 | 3.964 | 59.032 | 1.00 41.48 |
| MOTA | 3040 CE LYS B | 5 | 48.234 | 3.803 | 57.577 | 1.00 43.62 |
| ATOM | 3041 NZ LYS B | 5 | 49.215 | 3.025 | 56.781 | 1.00 42.53 |
| ATOM | 3042 C LYS B | 5. | 50.512 | 3.749 | 63.038 | 1.00 32.67 |
| ATOM | 3043 O LYS B | 5 | 51.012 | 2.995 | 63.878 | 1.00 25.78 |
| ATOM | 3044 N LEU B | 6 | 49.937 | 4.906 | 63.343 | 1.00 27.07 |
| MOTA | 3045 CA LEU B | 6 | 49.821 | 5.379 | 64.712 | 1.00 31.09 |
| ATOM | 3046 CB LEU B | 6 | 50.596 | 6.696 | 64.896 | 1.00 30.13 |
| ATOM | 3047 CG LEU B | 6 | 50.691 | 7.340 | 66.285 | 1.00 28.09 |
| ATOM | 3048 CD1 LEU B | 6 | 49.333 | 7.827 | 66.728 | 1.00 38.87 |
| MOTA | 3049 CD2 LEU B 3050 C LEU B | 6 | 51.248 | 6.338 | 67.282 | 1.00 24.87 |
| MOTA | | 6 | 48.324 | 5.594 | 64.924 | 1.00 29.52 |
| MOTA | | 6 | 47.669 | 6.287 | 64.149 | 1.00 33.36 |
| ATOM | | 7 7 | 47.777 | 4.975 | 65.960 | 1.00 28.02 |
| ATOM | | 7 | 46.361 | 5.111 | 66.250 | 1.00 23.83 |
| ATOM ATOM | 3054 CB ILE B 3055 CG2 ILE B | 7 . | 45.736 44.309 | | 66.670 | 1.00 25.11 |
| ATOM | 3056 CG1 ILE B | 7 | 45.690 | | 67.127 | 1.00 23.59 |
| ATOM | 3057 CD1 ILE B | 7 | 47.021 | | 65.477 | 1.00 31.00 |
| ATOM | 3058 C ILE B | 7 | 46.179 | | 64.906 67.363 | 1.00 38.60 |
| ATOM | 3059 O ILE B | 7 | 46.766 | | 68.430 | 1.00 26.49 1.00 26.68 |
| | - 200 2 | | | v. vu 3 | 00.430 | 1.00 20.00 |

| ATOI | M 3060 | N GLY | B 8 | | 45.37 | 2 7.15 | 1 67 10 | _ |
|--------|---------------------|----------|-------|---|--------|----------|----------------|--------------|
| ATON | 4 3061 | CA GLY | | | | | | 6 1.00 29.51 |
| ATON | | | | | 45.15 | | 0 68.11 | 7 1.00 30.28 |
| | | C GLY | | | 44.21 | 7 9.27 | 3 67.66 | 7 1.00 28.79 |
| ATON | 1 3063 | O GLY | B 8 | | 43.62 | | | |
| ATOM | 1 3064 | N THR | B 9 | | 44.08 | | | |
| ATOM | f ₋ 3065 | CA THR | - | | | | | |
| | | | | | 43.23 | | 8 68.23 | B 1.00 29.37 |
| ATOM | | CB THR | | | 41.74 | | 4 68.313 | |
| ATOM | 1 3067 | OG1 THR | B 9 | | 40.95 | | 7 60 01 | |
| ATOM | 3068 | CG2 THR | В 9 | | | 1 10 20 | | |
| - | | C min | 5 5 | | 41.43 | | 3 69.637 | 7 1.00 33.42 |
| ATOM | | C _THR | | | 43.47 | | 6 69.302 | |
| ATOM | 3070 | O THR | B 9 | | 43.88 | | 3 70.416 | |
| ATOM | 3071 | n leu | B. 10 | | 43.22 | 8 13.75 | | |
| ATOM | 3072 | CA LEU | | | | | | |
| | | | | | 43.39 | | 0 69. 914 | F 1.00 34.75 |
| ATOM | | CB LEU | | | 43.38 | 1 16.18 | 9 69.190 | |
| ATOM | 3074 | CG LEU | B 10 | | 44.60 | 5 16.57 | | |
| ATOM | 3075 | CD1 LEU | | | 44.96 | | | |
| ATOM | | CD2 LEU | | | | | | |
| | | | | | 44.31 | | | 1.00 34.99 |
| ATOM | | C LEU | | | 42.272 | 2 14.809 | 70.945 | |
| ATOM | 3 07 8 (|) LEU | B 10 | | 42.415 | | | |
| ATOM | 3079 N | N ASP | | | | | | |
| ATOM | | | | | 41.158 | | | |
| | | | | | 40.011 | 14.098 | 71.501 | 1.00 33.08 |
| MOTA | | CB ASP | B 11 | | 38.928 | 13.167 | | |
| ATOM | 3082 C | G ASP | B 11 | | 38.372 | | | , |
| ATOM | 3083 C | D1 ASP | | | | | | 1.00 43.14 |
| ATOM | | D2 ASP | | | 38.013 | | | 1.00 42.22 |
| | | | | | 38.281 | | 68.681 | 1.00 45.58 |
| ATOM | 3085 C | | | | 40.358 | 13.654 | 72.919 | 1.00 32.19 |
| ATOM | 3086 O | ASP F | 3 11 | | 39.688 | | | 2.00 32.13 |
| ATOM | 3087 N | TYR E | | | 41.386 | 12.000 | 73.073 | 1.00 23.44 |
| ATOM | 3088 C | | | | | | 73.06 6 | 1.00 28.02 |
| | | | | | 41.770 | | 74.402 | 1.00 32.00 |
| ATOM | 3089 C | | | | 43.011 | 11.476 | 74.363 | 1.00 28.67 |
| MOTA | 3090 C | G TYR E | 12 | • | 42.821 | 10.108 | 73.737 | 1 00 25 33 |
| MOTA | 3091 C | D1 TYR B | | | 43.338 | | | 1.00 25.33 |
| ATOM | | E1 TYR B | | | | 9.823 | 72.475 | 1.00 23.74 |
| | | | | | 43.235 | 8.546 | 71.924 | 1.00 22.85 |
| ATOM | | D2 TYR B | | | 42.183 | 9.077 | 74.436 | 1.00 21.93 |
| MOTA | 3094 CI | E2 TYR B | 12 | | 42.074 | 7.793 | 73.889 | 1.00 21.99 |
| ATOM | 3095 C2 | | | | 42.605 | 7.538 | | |
| ATOM | 3096 OF | _ | | | | | 72.640 | 1.00 22.99 |
| | | | | | 42.532 | 6.273 | 72.109 | 1.00 18.79 |
| ATOM | 3097 C | TYR B | 12 | | 42.054 | 13.567 | 75.319 | 1.00 32.74 |
| ATOM | 3098 O | TYR B | 12 | | 41.986 | 13.450 | 76.542 | 1.00 23.85 |
| MOTA | 3099 N | GLY B | 13 | | 42.374 | 14.710 | 74.720 | |
| ATOM | 3100 CA | GLY B | 13 | | | 15.710 | | 1.00 26.96 |
| ATOM | 3101 C | | | | 42.658 | 15.900 | 75.501 | 1.00 34.92 |
| | | GLY B | 13 | | 41.452 | 16.396 | 76.277 | 1.00 36.82 |
| ATOM | 3102 0 | GLY B | 13 | | 41.580 | 17.228 | 77.176 | 1.00 34.10 |
| MOTA | 3103 · N | LYS B | 14 | | 40.279 | 15.875 | 75.929 | |
| ATOM | 3104 CA | LYS B | 14 | | 39.031 | | | 1.00 37.23 |
| ATOM | 3105 CB | | | | | 16.247 | 76.584 | 1.00 41.77 |
| | | | 14 | | 37.925 | 16.406 | 75.537 | 1.00 45.82 |
| ATOM | 3106 CG | | 14 | | 38.110 | 17.585 | 74.579 | 1.00 51.38 |
| MOTA | 3107 CD | LYS B | 14 | | 37.805 | 18.939 | 75.241 | 1.00 57.78 |
| ATOM | 3108 CE | LYS B | 14 | | 38.752 | | | |
| ATOM | 3109 NZ | LYS B | | | | 19.285 | 76.388 | 1.00 58.82 |
| | | | 14 | | 38.387 | 20.568 | 77.070 | 1.00 55.06 |
| atom | 3110 C | LYS B | 14 | | 38.591 | 15.226 | 77.627 | 1.00 39.50 |
| ATOM | 3111 o | LYS B | 14 | | 37.546 | 15.385 | 78.252 | 1.00 35.54 |
| MOTA . | 3112 N | TYR B | 15 | | 39.395 | | | 1.00 33.34 |
| ATOM | 3113 CA | | | | 39.393 | 14.186 | 77.815 | 1.00 40.97 |
| | | TYR B | 15 | | 39.070 | 13.128 | 78.768 | 1.00 44.15 |
| ATOM | 3114 CB | TYR B | 15 | | 38.863 | 11.827 | 77.990 | 1.00 44.42 |
| ATCM | 3115 CG | TYR B | 15 | | 37.850 | 11.972 | 76.876 | 1.00 42.02 |
| ATOM | 3116 CD1 | TYR B | 15 | | 38.064 | | | 1 00 44 02 |
| ATOM | 3117 CE1 | | | | | 11.389 | 75.634 | 1.00 41.06 |
| - | | | 15 | | 37.138 | 11.530 | 74.603 | 1.00 42.76 |
| ATOM | 3118 CD2 | | 15 | | 36.678 | 12.703 | 77.065 | 1.00 42.99 |
| ATOM | 3119 CE2 | | 15 | | 35.748 | 12.851 | 76.048 | 1.00 43.30 |
| ATOM | 3120 CZ | TYR B | 15 | | 35.984 | | | |
| | 3121 OH | TYR B | 15 | | | 12.261 | 74.816 | 1.00 45.49 |
| ATCM | | | | | 35.066 | 12.403 | 73.801 | 1.00 45.69 |
| ATOM | 3122 C | TYR B | 15 | | 40.151 | 12.944 | 79.838 | 1.00 43.48 |
| ATOM | 3123 O | TYR B | 15 | | 40.519 | 11.819 | | 1.00 41.20 |
| ATCM | 3124 N | ARG B | 16 | | 40.647 | | | |
| | 3125 CA | ARG B | 16 | | | 14.052 | | 1.00 43.01 |
| ATOM | (7 | A.C D | 40 | 4 | 41.686 | 14.012 | 81.410 | 1.00 43.70 |
| | | | | | | | | |

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Figure 18-48

| MOTA | 1 3126 | CB ARG | B 16 | 42.25 | 0 15.410 | 81.66 | 3 1.00 49.13 |
|--------|---------|----------|------|--------|----------|-------------------|--------------|
| ATOM | 4 3127 | CG ARG | B 16 | 42.65 | | | |
| ATOM | 1 3128 | CD ARG | | 43.85 | | | |
| ATOM | | NE ARG | | | | | |
| ATOM | | | _ | 44.30 | | | 3 1.00 62.87 |
| | | CZ ARG | | 44.62 | 3 17.818 | 3 78 <i>.</i> 951 | 1.00 64.92 |
| ATOM | | NH1 ARG | B 16 | 44.55 | 5 18.308 | 80.182 | |
| ATOM | 3132 | NH2 ARG | B 16 | 45.02 | | | |
| ATOM | 3133 | C ARG | | 41.093 | | | |
| ATOM | | O ARG | | | | | |
| ATOM | | | | 39.882 | | | |
| | | N TYR | | 41.949 | 13.056 | 83.628 | |
| MOTA | | CA TYR | | 41.494 | | | |
| ATOM | 3137 | CB TYR | B 17 | 42.500 | | | |
| ATOM | 3138 | CG TYR | | 42.413 | | | |
| ATOM | | CD1 TYR | B 17 | | | | |
| ATOM | | | | 42.530 | | | |
| | | | | 42.502 | | 83.287 | 1.00 21.42 |
| ATOM | | CD2 TYR | 2-1 | 42.258 | 9.196 | 85.984 | 1.00 24.67 |
| MOTA | | CE2 TYR | B 17 | 42.229 | 7.873 | 85.556 | |
| ATOM | 3143 | CZ TYR : | B 17 | 42.355 | | | 1.00 27.13 |
| MOTA | 3144 | OH TYR I | | 42.371 | | | |
| MOTA | 3145 | C TYR I | | | | | |
| ATOM | | | | 41.377 | | 85.765 | 1.00 38.94 |
| | | O TYR I | _ | 41.947 | 14.951 | 85.391 | 1.00 39.65 |
| ATOM | | N PRO I | | 40.647 | 13.893 | 86.891 | 1.00 41.27 |
| ATOM | 3148 | CD PRO E | 3 18 | 39.958 | 12.728 | 87.462 | 1.00 43.62 |
| MOTA | 3149 | CA PRO E | 3 18 | 40.448 | 15.058 | 87.762 | |
| ATOM | 3150 | CB PRO E | | 39.648 | | | 1.00 45.33 |
| MOTA | | CG PRO E | | | 14.473 | 88.928 | 1.00 44.09 |
| ATOM | | | | 40.096 | 13.015 | 88.933 | 1.00 49.22 |
| | | | | 41.702 | 15.809 | 88.221 | 1.00 45.86 |
| MOTA | | O PRO B | | 42.789 | 15.244 | 88.317 | 1.00 45.44 |
| MOTA | | N LYS B | 19 . | 41.506 | 17.095 | 88.507 | 1.00 48.42 |
| MOTA | 3155 (| CA LYS B | 19 | 42.535 | 18.040 | 88.952 | 1.00 51.03 |
| ATOM | 3156 (| CB LYS B | 19 | 41.873 | 19.122 | 89.814 | |
| ATOM | | CG LYS B | | 40.630 | | | 1.00 56.35 |
| ATOM | | D LYS B | _ | | 18.657 | 90.563 | 1.00 65.69 |
| | _ | | | 40.894 | 17.441 | 91.423 | |
| ATOM | | E LYS B | 19 | 39.602 | 16.882 | 91.9 99 | 1.00 71.85 |
| MOTA | | NZ LYS B | 19 | 39.825 | 15.603 | 92.731 | 1.00 72.79 |
| MOTA | 3161 0 | LYS B | 19 | 43.830 | 17.593 | 89.639 | 1.00 48.62 |
| MOTA | 3162 C | LYS B | 19 | 44.912 | 18.009 | 89.235 | |
| ATOM | 3163 N | ASN B | 20 | 43.745 | | | |
| ATOM | | A ASN B | 20 | | 16.775 | 90.678 | 1.00 43.99 |
| ATOM | | | | 44.957 | 16.356 | 91.375 | 1.00 43.86 |
| | | | 20 | 44.740 | 16.440 | 92.890 | 1.00 45.92 |
| MOTA | | G ASN B | 20 | 44.418 | 17.848 | 93.355 | 1.00 49.44 |
| ATOM | 3167 O | D1 ASN B | . 20 | 45.194 | 18.779 | 93.138 | 1.00 47.72 |
| MOTA | 3168 N | D2 ASN B | 20 | 43.268 | 18.011 | 93.999 | 1.00 49.42 |
| ATOM | 3169 C | ASN B | 20 | 45.460 | 14.960 | | |
| ATOM | 3170 O | | 20 | | | 91.008 | 1.00 39.49 |
| ATOM | | | | 46.496 | 14.521 | 91.494 | 1.00 38.24 |
| | | | 21 | 44.729 | 14.274 | 90.140 | 1.00 36.93 |
| ATOM | 3172 C | | 21 | 45.091 | 12.923 | 8 723 | 1.00 33.57 |
| ATOM | 3173 C | B HIS B | 21 | 43.948 | 12.299 | 87.924 | 1.00 28.67 |
| ATOM | 3174 C | G HIS B | 21 | 44.068 | 10.817 | 88.750 | |
| ATCM | 3175 CI | D2 HIS B | 21 | 44.779 | | | |
| ATOM | | O1 HIS B | | | 10.076 | 87.867 | 1.00 26.15 |
| | | | 21 | 43.431 | 9.917 | 89.57 8 | 1.00 29.59 |
| ATOM | | E1 HIS B | 21 | 43.743 | 8.686 | 89.212 | 1.00 23.65 |
| ATOM | 3178 NE | E2 HIS B | 21 | 44.560 | 8.755 | 88.177 | 1.00 29.71 |
| atom | 3179 C | HIS B | 21 | 46.348 | 12.928 | 88.852 | 1.00 29.06 |
| MOTA | 3180 O | HIS B | 21 | 46.536 | 13.805 | | 1.00 25.00 |
| ATCM | 3181 N | PRO B | | | | 88.015 | 1.00 24.86 |
| | | | 22 | 47.225 | 11.937 | 89.035 | 1.00 30.50 |
| ATOM | | | 22 | 47.187 | 10.802 | 89.976 | 1.00 31.51 |
| ATOM | 3183 CA | | 22 | 48.446 | 11.880 | 88.231 | 1.00 29.58 |
| ATCM | 3184 CB | PRO B | 22 | 49.055 | 10.549 | 88.656 | 1.00 33.72 |
| ATOM | 3185 CG | | 22 | 43.658 | 10.489 | 90.124 | 1.00 31.07 |
| TOM | 3186 C | PRO B | 22 | 48.176 | | | |
| | 3187 0 | | | | 11.950 | 86.728 | 1.00.28.52 |
| ATOM | | PRO B | 22 | 48.989 | 12.474 | 85.972 | 1.00 31.85 |
| TOM | 3188 N | LEU B | 23 | 47.030 | 11.435 | 86.297 | 1.00 24.47 |
| TOM | 3189 CA | | 23 | 46.685 | | | 1.00 27.80 |
| ATOM . | 3190 CB | LEU B | 23 | 45.933 | | | 1.00 22.18 |
| HOT | 3191 CG | | 23 | 46.760 | | 84 556 | 1.00 29.32 |
| | , | | | 2000 | 8.852 | 84.556 | 1.00 29.32 |
| | | | | | | | |

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Figure 18-49

| | | | | | | | • | | | | |
|--------|-------|-----|-------|----|----|---|------------------|--------|-----------------|------|-------|
| ATOM | 3192 | cr | 1 LEC | JВ | 23 | | 45.868 | 7.628 | 84.402 | 1.00 | 24.94 |
| ATOM | 3193 | CD | 2 LET | JВ | 23 | | 47.805 | | 83.446 | | 24.80 |
| ATOM | 3194 | С | LĒU | | 23 | | 45.891 | | 84.367 | | 27.95 |
| ATOM | 3195 | | LEU | | 23 | | 45.166 | | 83.373 | | 24.42 |
| ATOM | 3196 | | LYS | | 24 | | 46.011 | | 85.018 | | 31.01 |
| MOTA | 3197 | | | | 24 | | 45.261 | | 84.530 | | 29.40 |
| ATOM | 3198 | | | | 24 | | 44.934 | 15.923 | 85.665 | | |
| ATOM | 3199 | | | | 24 | | 45.979 | 16.969 | | 1.00 | |
| ATOM | 3200 | | | | 24 | | | | 85.999 | | 33.54 |
| ATOM | 3201 | | LYS | | 24 | | 47.300 | 16.397 | 86.422 | | 39.10 |
| ATOM | 3202 | NZ | LYS | | 24 | | 48.109 48.224 | 17.466 | 87.152 | | 45.49 |
| ATOM | 3203 | c | LYS | | 24 | | | 18.737 | 86.380 | | 45.95 |
| ATOM | 3204 | õ | LYS | | 24 | | 46.039 | 15.653 | 83.425 | | 30.02 |
| ATOM | 3205 | Ŋ | ILE | | 25 | | 45.508 | 16.523 | 82.736 | | 28.82 |
| ATOM | 3205 | CA | | | | | 47.298 | 15.262 | 83.246 | | 25.93 |
| | 3207 | CB | ILE | | 25 | | 48.139 | 15.858 | 82.212 | | 29.48 |
| MOTA | 3208 | CG | | | 25 | | 49.641 | 15.528 | 82.409 | 1.00 | |
| MOTA | 3209 | CG: | | | 25 | | 50.126 | 16.033 | 83.775 | 1.00 | |
| ATOM | | | | | 25 | | 49.851 | 14.014 | 82.263 | 1.00 | |
| MOTA | 3210 | | | | 25 | | 51.310 | 13.584 | 82.188 | 1.00 | |
| ATOM | 3211 | 2 | ILE | | 25 | | 47.784 | 15.318 | 80.834 | | 30.08 |
| MOTA | 3212 | 0 | ILE | | 25 | | 47.263 | 14.210 | 80.704 | | 25.37 |
| ATOM | 3213 | N | PRO | | 26 | | 48.064 | 16.101 | 79.783 | | 29.19 |
| MOTA | 3214 | CD | PRO | | 26 | | 48.650 | 17.448 | 79.770 | | 32.47 |
| MOTA | 3215 | CA | PRO | | 26 | | 47.782 | 15.673 | 78.413 | | 29.52 |
| MOTA | 3216 | CB | PRO | | 26 | | 48.103 | 16.921 | 77.593 | | 29.84 |
| ATOM | 3217 | CG | PRO | | 26 | | 47.930 | 18.046 | 78.599 | | 36.40 |
| ATOM | 3218 | C | PRO | | 26 | | 48.789 | 14.561 | 78.137 | | 27.64 |
| ATOM | 3219 | 0 | PRO | | 26 | - | 49.920 | 14.620 | 78 .629 | | 23.08 |
| ATOM | 3220 | Ä | ARG | | 27 | | 48.403 | 13.557 | 77.360 | | 23.09 |
| ATOM | 3221 | CA | ARG | | 27 | | 49.326 | 12.469 | 77.072 | | 23.00 |
| ATOM | 3222 | CB | ARG | | 27 | | 48.987 | 11.264 | 77.962 | | 26.21 |
| MOTA | 3223 | CG | ARG | | 27 | | 49.101 | 11.617 | 79.449 | | 17.03 |
| MOTA | 3224 | CD | ARG | | 27 | | 48.663 | 10.507 | 80.416 | | 26.83 |
| ATOM | 3225 | NE | ARG | | 27 | | 49.586 | 9.375 | 80.502 | | 22.99 |
| ATOM | 3226 | CZ | ARG | | 27 | | 49.444 | 8.220 | 79.856 | | 25.06 |
| ATOM | 3227 | | ARG | | 27 | | 48.408 | 8.022 | 79.059 | 1.00 | |
| ATOM | 3228 | NH2 | | | 27 | | 50.336 | 7.253 | 80.027 | | 23.38 |
| ATOM | 3229 | Č | ARG | | 27 | | 49.329 | 12.097 | 75.595 | | 22.54 |
| ATOM | 3230 | 0 | ARG | | 27 | | 50.214 | 12.526 | 74.852 | | 21.86 |
| ATOM . | 3231 | N | VAL | | 28 | | 48.352 | 11.318 | 75.148 | | 20.64 |
| ATOM | 3232 | CA | VAL | | 28 | | 48.337 | 10.954 | 73.739 | | 26.57 |
| ATOM | 3233 | CB | VAL | | 28 | | 47.242 | 9.917 | 73.424 | | 30.92 |
| ATOM | 3234 | CG1 | VAL | | 28 | | 47.195 | 9.645 | 71.925 | | 27.04 |
| ATOM | 3235 | CG2 | VAL | | 28 | | 47.535 | 8.616 | 74.172 | | 25.45 |
| ATOM | 3236 | 2 | VAL | | 28 | | 48.150 | 12.189 | 72.866 | 1.00 | 28.02 |
| ATOM | 3:37 | 5 | VAL | | 28 | | 48.780 | 12.311 | 71.808 | | 30.88 |
| ATOM | 3.38 | N | SER | | 29 | | 47.298 | 13.112 | 73.304 | | 24.30 |
| ATOM | 3139 | CA | SER | | 29 | | 47.082 | 14.326 | 72.523 | | 29.48 |
| ATOM | 3240 | CB | SER | | 29 | | 45.939 | 15.169 | 73.110 | | 31.72 |
| ATOM | 3241 | OG | SER | | 29 | | 46.218 | 15.614 | 74.424 | | 34.55 |
| MOTA | 3242 | C | SER | | 29 | | 48.379 | 15.125 | 72.514 | | 30.81 |
| ATOM | 3243 | 0 | SER | | 29 | | 48.680 | 15.820 | 71.545 | | 28.85 |
| ATOM | 3244 | N | LEU | | 30 | | 49.157 | 15.003 | 73. 589 | 1.00 | 29.63 |
| ATOM | .3245 | CA | LEU | | 30 | | 50.427 | 15.721 | 73. 679 | | 31.59 |
| ATOM | 3246 | CB | LEU | | 30 | | 51.046 | 15.593 | 75.079 | 1.00 | 29.49 |
| ATOM | 3247 | CG | LEU . | | 30 | | 52.066 | 16.660 | 75.513 | | 34.37 |
| MOTA | 3248 | CD1 | LEU : | | 30 | | 52.937 | 16.083 | 76.610 | | 30.15 |
| MOTA | 3249 | CD2 | LEU | | 30 | | 52.951 | 17.098 | 74.357 | | 32.90 |
| MOTA | 3250 | 2 | LEU : | | 30 | | 51.371 | 15.085 | 7 2. 672 | | 25.90 |
| ATOM | 3251 | 2 | LEU : | | 30 | | 52.052 | 15.777 | 71.913 | 1.00 | 25.10 |
| ATOM | 3252 | И | LEU I | | 31 | | 51.404 | 13.756 | 72.675 | | 22.10 |
| ATOM | 3253 | CA | LEU I | В | 31 | | 52.268 | 13.013 | 71.764 | | 25.52 |
| ATOM | 3254 | CB | LEU I | | 31 | | 51.966 | 11.514 | 71.842 | 1.00 | 26.41 |
| ATOM | 3255 | CG | LEU I | | 31 | | 53.066 | 10.524 | 71.441 | 1.00 | |
| ATOM | 3256 | | LEU ! | | 31 | | 52,425 | 9.198 | 71.042 | 1.00 | 23.69 |
| ATOM | 3257 | CD2 | LEU ! | 3 | 31 | | 53.873 | 11.049 | 70.300 | 1.00 | |
| | | | | | | | | | | | |

| ATOM | 3258 | 3 C | LEU | 3 31 | | 52 010 | 12 420 | 70 775 | 1 00 05 30 |
|--------------|--------------|------|----------------|------|---|------------------|------------------|------------------|--------------------------|
| MOTA | 3259 | | LEU | | | 52.010 52.940 | | 70.335 | |
| ATOM | 3260 | | LEU | | | 50.741 | | | 1.00 21.03 |
| ATOM | 3261 | | | B 32 | | | | 69.933 | 1.00 21.27 |
| ATOM | 3262 | | | | | 50.364 | | 68.585 | 1.00 27.91 |
| ATOM | 3263 | | | | | 48.841 | | 68.408 | 1.00 26.60 |
| ATOM | 3264 | | 1-LEU | | | 48.195 | | 68.614 | 1.00 27.30 |
| | 3265 | | | | | 46.699 | | 68.321 | 1.00 31.60 |
| MOTA | 3266 | | | | | 48.837 | | 67.708 | |
| MOTA | | | LEU | | | 50.835 | | 68.242 | 1.00 26.07 |
| MOTA | 3267 | | LEU | | | 51.458 | | 67.205 | 1.00 22.45 |
| ATOM | 3268 | | ARG | | • | 50.545 | | 69.111 | 1.00 28.19 |
| ATOM | . 3269 | | | | | 50.962 | | 68.865 | 1.00 31.77 |
| MOTA | 3270 | | | | | 50.395 | 18.601 | 69.930 | 1.00 34.22 |
| MOTA | 3271 3272 | | | | | 48.887 | 18.740 | 69.904 | 1.00 40.33 |
| ATOM | 3273 | | | | | 48.420 | 19.713 | 70.970 | 1.00 47.67 |
| ATOM | | | | | | 46.977 | 19.931 | 70.924 | 1.00 56.24 |
| ATOM | 3274 | | | | | 46.330 | 20.505 | 69.912 | 1.00 60.10 |
| ATOM | 3275 | | 1 ARG | | | 46.997 | 20.929 | 68.845 | 1.00 63.11 |
| MOTA | 3276 3277 | | | | | 45.011 | 20.652 | 69.965 | 1.00 63.81 |
| ATOM | 3278 | 0 | ARG | | | 52.476 | 17.791 | 68.852 | 1.00 30.12 |
| ATOM | 3279 | N. | ARG : | | | 53.028 | 18.580 | 68.097 | 1.00 30.20 |
| ATOM | | | | B 34 | | 53.147 | 17.012 | 69.694 | 1.00 30.70 |
| MOTA | 3280 | CA | | B 34 | | 54.600 | 17.060 | 69.774 | 1.00 29.42 |
| ATOM | 3281 3282 | CB | PHE | | | 55.096 | 16.176 | 70.920 | 1.00 30.46 |
| MOTA | 3283 | CD: | PHE I PHE I | | | 56.556 | 16.358 | 71.248 | 1.00 28.56 |
| ATOM ATOM | 3284 | CD | | | | 57.001 | 17.515 | 71.885 | 1.00 26.92 |
| - | 3285 | | l PHE ! | | | 57.481 | 15.373 | 70.932 | 1.00 28.88 |
| ATOM ATOM | 3286 | | PHE I | | | 58.346 | 17.684 | 72.206 | 1.00 28.15 |
| MOTA | 3287 | CZ | PHE | | | 58.831 59.265 | 15.530 | 71.246 71.887 | 1.00 31.47 |
| MOTA | 3288 | c | PHE ' | | | 55.202 | 16.689 16.583 | 68.460 | 1.00 28.15 |
| ATOM | 3289 | ŏ | PHE I | | | 56.049 | 17.259 | 67.873 | 1.00 33.78 1.00 33.71 |
| ATOM | 3290 | N | LYS | | | 54.770 | 15.413 | 67.999 | 1.00 33.71 |
| ATOM | 3291 | CA | LYS | | | 55.294 | 14.880 | 66.753 | 1.00 28.83 |
| ATOM | 3292 | СВ | LYS E | | | 54.684 | 13.509 | 66.454 | 1.00 34.33 |
| ATOM | 3293 | CG | LYS E | | | 55.141 | 12.423 | 67.414 | 1.00 34.93 |
| ATOM | 3294 | CD | LYS E | | | 54.580 | 11.066 | 67.047 | 1.00 41.43 |
| ATOM | 3295 | CE | LYS E | | | 53.070 | 11.004 | 67.205 | 1.00 44.04 |
| ATOM | 3296 | NZ | LYS B | | • | 52.335 | 11.984 | 66.345 | 1.00 60.09 |
| ATOM | 3297 | С | LYS B | 35 | | 55.015 | 15.842 | 65.608 | 1.00 35.78 |
| MOTA | 3298 | 0 | LYS B | | | 55.869 | 16.061 | 64.752 | 1.00 33.39 |
| ATOM | 3299 | M | ASP B | 36 | | 53.823 | 16.426 | 65.602 | 1.00 32.32 |
| ATOM | 3300 | CA | ASP B | 36 | | 53.468 | 17.365 | 64.552 | 1.00 36.31 |
| ATOM | 3301 | CB | ASP B | 36 | | 52.015 | 17.800 | 64.698 | 1.00 42.56 |
| ATOM | 3302 | CG | ASP B | 36 | | 51.617 | 18.822 | 63.661 | 1.00 43.03 |
| MOTA | 3303 | OD1 | ASP B | 36 | | 51.812 | 18.544 | 62.461 | 1.00 79.17 |
| MOTA | 3304 | OD2 | ASP B | 36 | | 51.111 | 19.897 | 64.043 | 1.00 4.34 |
| ATOM | 3305 | С | ASP B | 36 | | 54.371 | 18.590 | 64.578 | 1.00 '6.14 |
| ATOM | 3306 | 0 | ASP B | 36 | | 54.764 | 19.099 | 63.534 | 1.00 32.40 |
| MOTA | 3307 | N | ALA B | . 37 | | 54.694 | 19.061 | 65.777 | 1.00 34.80 |
| ATOM | 3308 | CA | ALA B | 37 | | 55.554 | 20.226 | 65.924 | 1.00 36.82 |
| ATOM | 3309 | CB | ALA B | 37 | | 55.599 | 20.659 | 67.383 | 1.00 38.54 |
| MOTA | 3310 | С | ALA B | 37 | | 56.9 59 | 19.901 | 65.429 | 1.00 37.66 |
| ATOM | 3311 | 0 | ALA B | 37 | | 57.675 | 20.776 | 64.950 | 1.00 30.56 |
| ATOM | 3312 | N | MET B | 38 | | 57.346 | 18.635 | 65.541 | 1.00 37.42 |
| MOTA | 3313 | CA | MET 3 | 38 | | 58.670 | 18.192 | 65. 10 7 | 1.00.36.25 |
| ATOM | 3314 | CB | MET 3 | 38 | | 59.158 | 17.059 | 66.013 | 1.00 36.44 |
| ATOM | 3315 | CG | MET 3 | 38 | | 59.341 | 17.438 | 67.474 | 1.00 37.68 |
| MOTA | 3316 | SD | MET B | 38 | | 60.841 | 18.391 | 67.784 | 1.00 38.07 |
| ATOM | 3317 | CE . | MET 3 | 38 | | 62.093 | 17.228 | 67.300 | 1.00 30.98 |
| ATOM | 3318 | C | MET B | 38 | | 58.639 | 17.690 | 63.663 | 1.00 35.86 |
| ATOM | 3319 | 0 | MET B | 38 | | 59.659 | 17.262 | 63.130 | 1.00 32.69 |
| ATOM | 3320 | N- | ASN B | 39 | | 57.470 | 17.742 | 63.035 | 1.00 35.82 |
| atom | 3321 | CA | ASN B | 39 | | 57.321 | 17.262 | 61.661 | 1.00 42.75 |
| ATOM | 3322 | CB | ASN B | 39 | | 58.156 | 18.108 | 60.688 | 1.00 46.20 |
| MOTA | 3323 | CG | ASN B | 39 | | 57.670 | 19.543 | 60.591 | 1.00 47.57 |

| ATON | | OD1 ASN | B 39 | 56.52 | 4 19.801 | 60.212 | 2 1.00 48.78 |
|------|----------------|-----------|------|----------|----------|--------------------|--------------|
| ATOM | 1 3325 | ND2 ASN | B 39 | 58.54 | | | |
| ATOM | | C ASN | | | | | |
| ATOM | | | | 57.75 | | | |
| | | O ASN | | 58.46 | 5 15.416 | 60.639 | 1.00 35.75 |
| ATOM | | n leu | B 40 | 57.33 | 2 14.997 | 62.535 | |
| ATOM | 3329 | CA LEU | B 40 | 57.70 | | | |
| ATOM | 3330 | CB LEU | | 58.34 | | | |
| ATOM | | | | | | | |
| | | CG LEU | | 59.59 | | | 1.00 36.21 |
| ATOM | | CD1 LEU | B 40 | 60.148 | 3 13.648 | 65.573 | |
| ATOM | 3333 | CD2-LEU | B 40 | 60.646 | | | |
| ATOM | | C LEU | | 56.549 | | | |
| ATOM | | | | | | | |
| - | | D LEU | | 56.637 | 11.438 | 62.573 | 1.00 39.15 |
| ATOM | 3336 1 | N ILE | B 41 | 55.476 | 13.131 | | |
| MOTA | 3337 (| CA ILE : | | 54.340 | | 61.314 | |
| MOTA | 3338 | CB ILE | | 53.445 | | | 1.00 35.42 |
| ATOM | | G2 ILE | | | | 62.536 | |
| | | | | 52.793 | | 63.047 | |
| ATOM | | G1 ILE | | 52.367 | 10.980 | 62.141 | 1.00 32.68 |
| ATOM | 3341 (| CD1 ILE 1 | B 41 | 51.470 | 10.550 | 63.285 | 1.00 36.46 |
| ATOM | 3342 (| : ILE 1 | B 41 | 53.492 | | 60.229 | |
| ATOM | 3343 0 | | | | - " | | |
| | | | | 53.352 | | 60.183 | 1.00 40.24 |
| ATOM | | | | 52.943 | 12.114 | 59.345 | 1.00 39.55 |
| ATOM | 3345 C | A ASP I | 3 42 | 52.094 | 12.615 | 58.273 | 1.00 45.30 |
| ATOM | 3346 C | B ASP E | 3 42 | 52.569 | 12.119 | 56.901 | 1.00 45.93 |
| ATOM | 3347 C | G ASP E | | 53.972 | | 50.501 | |
| ATOM | | D1 ASP E | | | 12.584 | 56.564 | 1.00 47.09 |
| | | | | 54.244 | 13.799 | 56.686 | 1.00 46.60 |
| ATOM | | D2 ASP E | | 54.797 | 11.736 | 56.162 | 1.00 45.16 |
| ATOM | 3350 C | ÀSP E | 3 42 | 50.677 | 12.134 | 58.524 | 1.00 45.15 |
| ATOM | 3351 0 | ASP B | 42 | 50.467 | 11.051 | 59.069 | 1 00 47 06 |
| ATCM | 3352 N | | | 49.707 | | | 1.00 47.06 |
| ATOM | 3353 C | _ | | | 12.944 | 58.121 | 1.00 48.13 |
| | | _ | | . 48.303 | 12.618 | 58.312 | 1.00 50.50 |
| ATOM | 3354 C | | | 47.441 | 13.637 | 57.571 | 1.00 53.54 |
| ATOM | 3355 C | G GLUB | 43 | 45.961 | 13.505 | 57.840 | 1.00 59.52 |
| ATOM | 3356 CI | D GLU B | 43 | 45.155 | 14.518 | 57.065 | 1.00 64.03 |
| ATOM | 3357 O | E1 GLU B | | | | | |
| ATOM | | E2 GLU B | 43 | | 14.535 | 57.215 | 1.00 68.54 |
| | | | | 45.765 | 15.298 | 56.301 | 1.00 66.95 |
| ATOM | 3359 C | GLU B | 43 | 47.972 | 11.205 | 57.836 | 1.00 47.81 |
| ATOM | 3 360 O | GLU B | 43 | 47.092 | 10.547 | 5 8.390 | 1.00 49.67 |
| ATOM | 3361 N | LYS B | 44 | 48.690 | 10.744 | 56.817 | 1.00 46.21 |
| ATOM | 3362 C | | 44 | 48.484 | 9.409 | | 1.00 40.21 |
| MOTA | 3363 CE | | | | | 56.251 | 1.00 48.28 |
| | | | 44 | 49.207 | 9.311 | 54.894 | 1.00 49.96 |
| MOTA | 3364 CC | | 44 | 49.639 | 7.903 | 54.470 | 1.00 52.18 |
| MOTA | 3365 CI | LYSB | 44 | 50.970 | 7.532 | 55.127 | 1.00 61.03 |
| ATOM | 3366 CE | LYS B | 44 | 51.399 | 6.095 | 54.844 | 1.00 62.80 |
| ATOM | 3367 NZ | LYS B | 44 | 50.511 | 5.098 | | |
| ATOM | 3368 C | LYS B | | | | 55.510 | 1.00 65.34 |
| | | | 44 | 48.899 | 8.249 | 57.161 | 1.00 45.92 |
| ATOM | 3369 o | LYS B | 44 | 48.418 | 7.127 | 57.00 9 | 1.00 41.30 |
| MOTA | 3370 N | GLU B | 45 | 49.797 | 8.517 | 58:100 | 1.00 42.18 |
| ATOM | 3371 CA | GLU B | 45 | 50.268 | 7.486 | 59.014 | 1.00 38.41 |
| ATOM | 3372 CB | | 45 | 51.684 | | | |
| ATOM | 3373 CG | | | | 7.812 | 59.468 | 1.00 33.73 |
| | | | 45 | 52.694 | 7.887 | 58.351 | 1.00 37.58 |
| ATOM | 3374 CD | | 45 | 53.998 | 8.504 | 58.813 | 1.00 34.34 |
| MOTA | 3375 OE | 1 GLU B | 45 | 53.997 | 9.699 | 59.176 | 1.00 38.04 |
| ATOM | 3376 OE | 2 GLU B | 45 | 55.020 | 7.799 | 58.821 | 1.00 33.37 |
| ATOM | 3377 C | GLU B | 45 | 49.368 | | | |
| | | | | | 7.403 | 60.238 | 1.00 36.86 |
| ATOM | 3378 0 | GLU B | 45 | 49.461 | 6.462 | 61.032 | 1.00 34.98 |
| atom | 3379 N | LEU B | 46 | 48.489 | 8.386 | 60.386 | 1.00 30.86 |
| MOTA | 3380 CA | LEU B | 46 . | 47.608 | 8.438 | 61.545 | 1.00 30.65 |
| ATOM | 3381 CB | LEU B | 46 | 47.501 | 9.889 | 62.019 | 1.00 32.74 |
| ATOM | 3382 CG | LEU B | 46 | | | | |
| | | | | 46.642 | 10.163 | 63.250 | 1.00 34.76 |
| ATOM | | L LEU B | 46 | 47.189 | 9.379 | 64.425 | 1.00 32.24 |
| atom | 3384 CD2 | LEU B | 46 | 46.639 | 11.656 | 63.548 | 1.00 33.94 |
| ATOM | 3385 C | LEU B | 46 | 46.212 | 7.861 | 61.318 | 1.00 31.36 |
| ATOM | 3386 0 | LEU B | 46 | 45.530 | | 60.363 | |
| | 3387 N | ILE B | 47 | | 8.218 | | 1.00 31.78 |
| ATOM | | | | 45.801 | 6.957 | 62.203 | 1.00 31.18 |
| ATOM | 3388 CA | ILE B | 47 | 44.479 | 6.338 | 62.139 | 1.00 29.36 |
| ATOM | 3389 CB | ILE B | 47 | 44.564 | 4.802 | 62.258 | 1.00 28.62 |
| | | | | | | | |

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Figure 18-52

| MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 339 339 339 339 339 339 339 340 340 | 1 CG1 ILE 2 CD1 ILE 3 C ILE 4 O ILE 5 N LYS 6 CA LYS 7 CB LYS 8 CG LYS 9 CD LYS 0 CE LYS 1 NZ LYS | B 47 B 47 B 47 B 47 B 48 B 48 B 48 B 48 B 48 B 48 | 43.161 45.266 45.419 43.659 44.063 42.514 41.662 40.517 39.607 38.535 37.657 38.451 | 4.230 2.722 6.875 6.755 7.475 8.037 8.840 9.514 10.361 11.074 11.991 | 61.028 61.054 63.303 64.461 | 1.00 29.42 1.00 31.12 1.00 32.22 1.00 31.17 1.00 28.39 1.00 36.32 1.00 43.08 1.00 44.38 1.00 45.91 |
|---|---|---|--|--|--|--------------------------------------|--|
| . ATOM | 3402 3403 | | | 41.095 | | 64.937 | |
| ATOM | 3404 | | | 40.524 41.260 | | 64.457 66.244 | |
| ATOM | 3405 | | | 40.770 | | 67.232 | |
| MOTA MOTA | 3406 3407 | | | 41.146 | | 68.642 | |
| ATOM | 3408 | | | 42.539 39.248 | 6.858 6.054 | 68.777 67.160 | 1.00 31.79 1.00 29.07 |
| ATOM | 3409 | | | 38.565 | 7.034 | 66.879 | 1.00 29.07 |
| MOTA | 3410 | | | 38.723 | 4.859 | 67.409 | 1.00 26.13 |
| ATOM ATOM | 3411 3412 | | | 37.278 | 4.658 | 67.430 | 1.00 24.24 |
| ATOM | 3413 | | | 36.810 37.231 | 3.700 2.233 | 66.323 66.507 | 1.00 25.03 1.00 26.54 |
| ATOM | 3414 | | | 36.570 | 1.340 | 65.452 | 1.00 26.34 |
| ATOM | 3415 | | | 37.006 | -0.058 | 65.504 | 1.00 25.13 |
| ATOM ATOM | 3416 3417 | CZ ARG E | | 36.700 | -0.924 | 66.468 | 1.00 26.09 |
| ATOM | 3418 | NH2 ARG B | | 35.941 37.157 | -0.558 -2.168 | 67.497 66.402 | 1.00 23.42 1.00 23.91 |
| ATOM | 3419 | C ARG B | 50 | 36.937 | 4.037 | 68.775 | 1.00 23.83 |
| ATOM ATOM | 3420 3421 | O ARG B | | 37.782 | 3.392 | 69.403 | 1.00 21.60 |
| ATOM | 3422 | N PRO B | 51 51 | . 35.700 34.554 | 4.223 | 69.243 68.688 | 1.00 22.99 1.00 25.09 |
| ATOM | 3423 | CA PRO B | 51 | 35.338 | 3.628 | 70.530 | 1.00 25.48 |
| ATOM | 3424 | CB PRO B | 51 | 33.949 | 4.217 | 70.802 | 1.00 26.32 |
| ATOM ATOM | 3425 3426 | CG PRO B | 51 51 | 33.936 | 5.503 | 69.953 70.325 | 1.00 28.65 |
| ATOM | 3427 | O PRO B | 51 | 35.264 35.142 | 2.118 | 69.194 | 1.00 26.73 1.00 18.87 |
| ATOM | 3428 | N ALA B | 52 | 35.355 | 1.359 | 71.408 | 1.00 23.64 |
| ATOM ATOM | 3429 3430 | CA ALA B | 52 | 35.237 | -0.083 | 71.291 | 1.00 23.27 |
| ATOM | 3431 | C ALA B | 52 52 | 35.811 33.733 | -0.757 -0.324 | 72.521 71.223 | 1.00 26.31 1.00 25.25 |
| ATOM | 3432 | O ALA B | 52 | 32.950 | 0.515 | 71.677 | 1.00 23.23 |
| ATOM | 3433 | N THR B | 53 | 33.321 | -1.447 | 70.651 | 1.00 22.77 |
| ATOM ATOM | 3434 3435 | CA THR B | 53 · 53 | 31.900 | -1.760 | 70.596 | 1.00 26.90 |
| ATOM | 3436 | OG1 THR B | 53 | 31.567 32.305 | -2.732 -3.950 | 69.456 69.642 | 1.00 30.00 1.00 25.59 |
| ATOM | 3437 | CG2 THR B | 53 | 31.917 | -2.117 | 68.103 | 1.00 23.33 |
| MOTA | 3438 | C THR B | 53 | 31.579 | -2.445 | 71.916 | 1.00 30.41 |
| MOTA MOTA | 3439 3440 | O THR B N LYS B | 53 54 | 32.484 | -2.917 -2.504 | 72.609 72.268 | 1.00 26.13 1.00 29.12 |
| ATOM | 3441 | CA LYS B | 54 | 29.909 | -3.140 | 73.514 | 1.00 29.12 |
| ATOM | 3442 | CB LYS B | 54 | 28.396 | -3.027 | 73.720 | 1.00 32.78 |
| MOTA | 3443 3444 | CG LYS B | 54 | 27.947 | -3.351 | 75.131 | 1.00 34.85 |
| ATOM ATOM | 3445 | CE LYS B | 54 54 | 26.445 26.008 | -3.204 -3.366 | 75.268 76.709 | 1.00 41.13 1.00 43.39 |
| ATOM | 3446 | NZ LYS B | 54 | 26.464 | -2.257 | 77.582 | 1.00 47.39 |
| ATOM | 3447 | C LYS B | 54 | 30.329 | -4.603 | 73.442 | 1.00.29.10 |
| ATOM ATOM | 3448 3449 | O LYS B | 54 55 | 30.779 30.196 | -5.183 | 74.430 72.256 | 1.00 26.71 |
| ATOM | 3450 | CA GLU B | 55 | 30.196 | -5.187 -6.577 | 72.236 | 00 23.97 1.00 28.08 |
| ATCM | 3451 | CB GLU B | 55 | 30.288 | -6.965 | 70.579 | 1.00 24.82 |
| ATOM | 3452 | CG GLU B | 55 55 | 30.671 | -8.400 | 70.237 | 1.00 33.40 |
| ATOM ATOM | 3453 3454 | CD GLU B OE1 GLU B | 55 55 | 30.453 30.638 | -8.737 -9.913 | 68.767 68.394 | 1.00 38.49 1.00 41.24 |
| ATOM | 3455 | OE2 GLU B | 55 | 30.101 | -7.833 | 67.984 | 1.00 40.02 |
| | | | | | | | |

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| ATOM | 3456 | 5 C | GLU | B 55 | | 32.066 | -6.808 | 72.345 | 1.00 25.82 |
|---------------------|------|------|---------|----------|---|--------|---------|-------------|------------|
| ATOM | 3457 | 7 0 | GLU | B 55 | | 32.429 | | 73.033 | |
| | | | | | | | | | 1.00 23.83 |
| MOTA | 3458 | | GLU | B 56 | | 32.931 | -5.938 | 71.835 | 1.00 25.04 |
| ATOM | 3459 | C.F | A GLU | B 56 | | 34.365 | -6.079 | 72.093 | 1.00 25.30 |
| ATOM | 3460 | | | | | 35.141 | | | |
| | | | | | | | | 71.334 | 1.00 24.31 |
| ATOM- | 3461 | . CG | GLU | B 56 | | 34.866 | -5.039 | 69.836 | 1.00 32.15 |
| ATOM | 3462 | CI | GLU | B 56 | | 35.512 | -3.903 | 69.073 | 1.00 31.43 |
| | 3463 | | | | | | | | |
| ROTE | | | | | | 35.486 | | 69.568 | 1.00 28.54 |
| $MOT_{f_{\bullet}}$ | 3464 | O.E | :2 GLU | B 56 | | 36.012 | -4.147 | 67.959 | 1.00 28.89 |
| ATOM | 3465 | С | GLU | | | 34.653 | | 73.595 | 1.00 28.88 |
| | | | | | | | | | |
| ATOM | 3466 | | GLU | B 56 | | 35.450 | -6.766 | 74.137 | 1.00 25.07 |
| ATOM | 3467 | N | LEU | B. 57 | | 33.996 | -5.050 | 74.272 | 1.00 24.52 |
| MOTA | 3468 | CA | LEU | | - | 34.203 | | 75.702- | |
| | | | | | | | | | 1.00 27.34 |
| ATOM | 3469 | CB | LEU | B 57 | | 33.416 | -3.694 | 76.231 | 1.00 22.79 |
| ATOM | 3470 | CG | LEU | B 57 | | 33.859 | -2.320 | 75.722 | 1.00 23.57 |
| ATOM | 3471 | CD | | | | 33.008 | | 76.366 | |
| | | | | | | | | | 1.00 22.27 |
| MOTA | 3472 | CD | | | | 35.342 | -2.089 | 76.061 | 1.00 17.24 |
| MOTA | 3473 | С | LEU | B 57 | | 33.785 | -6.144 | 76.452 | 1.00 26.92 |
| ATOM | 3474 | 0 | LEU | | | | | | |
| | | | | | | 34.458 | -6.568 | 77.396 | 1.00 24.06 |
| MOTA | 3475 | N | LEU | B 58 | | 32.670 | -6.732 | 76.029 | 1.00 23.35 |
| MOTA | 3476 | CA | LEU : | B 58 | | 32.154 | -7.931 | 76.674 | 1.00 25.60 |
| ATOM | 3477 | CB | LEU | | | | | 76.221 | |
| | | | | | | 30.718 | -8.207 | | 1.00 28.50 |
| ATOM | 3478 | CG | LEU 1 | B 58 | | 29.734 | -7.110 | 76.649 | 1.00 30.91 |
| ATOM | 3479 | CD: | 1 LEU 1 | B 58 | | 28.323 | -7.468 | 76.212 | 1.00 28.93 |
| ATOM | 3480 | CD: | | | | | | | |
| | | | | | | 29.794 | -6.945 | 78.157 | 1.00 33.44 |
| ATOM | 3481 | С | LEU 1 | 3 58 | | 33.027 | -9.153 | 76.446 | 1.00 24.59 |
| ATOM | 3482 | 0 | LEU I | 3 58 | | 32.760 | -10.216 | 76.991 | 1.00 19.76 |
| ATOM | 3483 | N | LEU I | | | | | | |
| | | | | | | 34.065 | -9.006 | 75.630 | 1.00 23.99 |
| MOTA | 3484 | CA | LEU I | 3 59 | | 34.988 | -10.108 | 75.411 | 1.00 25.11 |
| ATOM | 3485 | CB | LEU I | 3 59 | | 36.018 | -9.757 | 74.332 | 1.00 21.64 |
| ATOM | 3486 | CG | LEU E | | | 35.483 | -9.652 | 72.905 | 1.00 24.24 |
| | | | | | | | | | |
| MOTA | 3487 | CD | | | | 36.585 | -9.177 | 71.975 | 1.00 24.25 |
| MOTA | 3488 | CD2 | LEU E | 3 59 | | 34.957 | -11.014 | 72.468 | 1.00 19.91 |
| ATOM | 3489 | С | LEU E | 59 | | 35.699 | -10.371 | 76.733 | 1.00 23.84 |
| | | | | | | | | | |
| MOTA | 3490 | О | LEU E | | | | -11.489 | 76.992 | 1.00 19.39 |
| ATOM | 3491 | N | PHE E | 60 | | 35.793 | -9.344 | 77.577 | 1.00 21.80 |
| ATOM | 3492 | CA | PHE E | 60 | | 36.462 | -9.510 | 78.876 | 1.00 23.08 |
| | 3493 | CB | | | | | | | |
| atom | | | PHE E | | | 37.809 | -8.770 | 78.908 | 1.00 18.22 |
| ATOM | 3494 | CG | PHE E | 60 | | 38.544 | -8.906 | 80.230 | 1.00 21.72 |
| ATOM | 3495 | CD1 | PHE B | 60 | | 38.975 | -10.157 | 80.680 | 1.00 19.23 |
| | 3496 | CD2 | | | | | | | |
| ATOM | | | | | | 38.757 | -7.791 | 81.048 | 1.00 17.75 |
| ATOM | 3497 | CE1 | PHE B | 60 | | 39.602 | -10.301 | 81.927 | 1.00 18.80 |
| ATOM | 3498 | CE2 | PHE B | 60 | | 39.384 | -7.923 | 82.297 | 1.00 19.23 |
| | 3499 | CZ | PHE B | | | | | | |
| ATOM | | | | | | 39.807 | -9.184 | 82.737 | 1.00 16.10 |
| ATOM | 3500 | С | PHE B | 60 | | 35.648 | -9.069 | 80.083 | 1.00 21.58 |
| ATOM | 3501 | 0 | PHE B | 60 | | 35.508 | -9.822 | 81.040 | 1.00 22.21 |
| ATOM | 3502 | N | HIS B | 61 | | 35.128 | -7.847 | 80.055 | 1.00 20.65 |
| | | | | | | | | | |
| ATOM | 3503 | CA | HIS B | 61 | | 34.362 | -7.336 | 81.184 | 1.00 23.32 |
| ATOM | 3504 | CB | HIS B | 61 | | 34.422 | -5.807 | 81.229 | 1.00 27.60 |
| ATOM | 3505 | CG | HIS B | 61 | | 35.800 | -5.259 | 81.440 | 1.00 31.83 |
| | | | | | | | | | - |
| ATOM | 3506 | CD2 | HIS B | 61 | | 36.466 | -4.940 | 82.575 | 1.00 26.86 |
| ATOM | 3507 | ND1 | HIS B | 61 | | 36.669 | ~5.003 | 80.401 | 1.00 34.35 |
| ATOM | 3508 | | HIS B | 61 | | 37.810 | -4.546 | 80.887 | 1.00 34.78 |
| | | | | | | | | | |
| ATOM | 3509 | | HIS B | 61 | | 37.713 | -4.499 | 82.204 | 1.00 36.27 |
| ATOM | 3510 | С | HIS B | 61 | | 32.902 | -7.775 | 81.198 | 1.00 28.04 |
| ATCM | 3511 | 0 | HIS B | 61 | | 32.349 | -8.167 | 80.176 | 1.00 25.70 |
| | | | | | | | | | |
| ATOM | 3512 | N | THR B | 62 | | 32.276 | -7.691 | 82.367 | 1.00 25.25 |
| ATOM | 3513 | CA | THR B | 62 | | 30.882 | -8.084 | 82.506 | 1.00 25.35 |
| ATOM | 3514 | CB | THR B | 62 | | 30.578 | -8.549 | 83.932 | 1.00 25.47 |
| | | | | | | | | | |
| ATOM | 3515 | OGI | THR B | 62 | | 30.783 | -7.462 | 84.843 | 1.00 28.62 |
| ATOM | 3516 | CG2 | THR B | 62 | | 31.482 | -9.701 | 84.315 | 1.00 21.32 |
| ATOM | 3517 | С | THR B | 62 | | 29.931 | -6.942 | 82.162 | 1.00 26.06 |
| | | | | | | | | | |
| ATOM | 3518 | 0 | THR B | 62 | | 30.287 | -5.771 | 82.254 | 1.00 24.14 |
| ATCM | 3519 | N | GLU B | 63 | | 28.718 | -7.305 | 81.759 | 1.00 28.01 |
| ATCM | 3520 | CA | GLU B | 63 | | 27.681 | -6.349 | 81.389 | 1.00 30.77 |
| | | CB | | 63 | | | | 81.114 | |
| ATCM | 3521 | ط | GLU B | . | | 26.374 | -7.094 | 0 T • T T # | 1.00 33.97 |

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| | | | | | | • | | | |
|--------------|--------------|---------|----------|--------------|---|------------------|------------------|--------------------------|--------------------------|
| MOTA | | | CG .GLU | B 63 | | 25.213 | -6.21 | 0 80.66 | 7 1.00 41.12 |
| ATOM | | | CD GLU | B 63 | | 25.189 | | | |
| ATOM | | | OE1 GLU | B 63 | | 24.361 | | | |
| ATOM | | | OE2 GLU | _ | | 25.992 | -6.64 | | |
| ATOM | | | C GLU | | | 27.436 | | | |
| ATOM | | | GLU | | | 27.381 | | | 2 1.00 25.13 |
| ATOM | | | N ASP | | | 27.272 | -5.834 | | 3 1.00 24.38 |
| ATOM | _ | | CA ASP | | | 27.010 | | | 7 1.00 29.27 |
| ATOM ATOM | | | CB ASP | _ | | 26.887 | | | 2 1.00 36.30 |
| ATOM | | | G ASP | | | 28.022 | | | |
| ATOM | | | | B 64 | | 29.128 | | - | |
| ATOM | | | | B 64 B 64 | | 27.812 | | | |
| ATOM | | | | | | 28.075 | | | |
| ATOM | | | | | | 27.768 29.332 | -2.806 | | |
| ATOM | | | A TYR | | | 30.420 | -4.373 | | |
| ATOM | | | B TYR | | • | 31.751 | -3.435 | | |
| ATOM | | | | | | 32.949 | -4.186 | | |
| ATOM | 354 | _ | D1 TYR | | • | 33.033 | -3.285 -2.328 | | |
| ATOM | 354 | 1 C | E1 TYR | | | 34.135 | -1.489 | | |
| ATOM | 354 | 2 C | D2 TYR | | | 34.004 | -3.382 | | |
| ATOM | 354 | 3 C | E2 TYR : | B 65 | | 35.116 | -2.544 | | 1.00 21.01 |
| ATOM | 354 | 4 C | Z TYR : | B 65 | | 35.172 | -1.601 | | |
| MOTA | 354 | | H TYR] | B 65 | | 36.262 | -0.775 | | |
| MOTA | 354 | | TYR I | - | | 30.392 | -2.373 | 84.146 | |
| ATOM | 354 | | TYR I | - | | 30.399 | -1.167 | 84.421 | 1.00 18.20 |
| MOTA | 3548 | | ILE I | | | 30.330 | -2.815 | 82.894 | 1.00 19.49 |
| ATOM | 3549 | _ | | | ٠ | 30.305 | -1.870 | 81.786 | 1.00 19.68 |
| ATOM ATOM | 3550 3551 | | _ | | | 30.208 | -2.592 | 80.432 | 1.00 23.31 |
| ATOM | 3552 | | | | | 30.200 | -1.571 | 79.303 | 1.00 21.30 |
| ATOM | 3553 | | | | | 31.400 32.758 | -3.541 | 80.260 | 1.00 27.67 |
| ATOM | 3554 | | ILE E | | | 29.128 | ~2.839 | 80.291 | 1.00 29.29 |
| ATOM | 3555 | | ILE B | | | 29.294 | -0.909 0.309 | 81.940 | 1.00 26.99 |
| ATOM | 3556 | | ASN B | | | 27.939 | -1.447 | 81.8 48 82.198 | 1.00 23.36 |
| ATOM | 3557 | CA | | | | 26.782 | -0.580 | 82.363 | 1.00 24.98 1.00 27.70 |
| ATOM | 3558 | CB | ASN B | 67 | | 25.492 | ~1.389 | 82.580 | 1.00 25.58 |
| ATOM | 3559 | | | 67 | | 25.081 | -2.183 | 81.341 | 1.00 26.91 |
| MOTA | 3560 | | | 67 | | 25.199 | -1.701 | 80.220 | 1.00 31.48 |
| MOTA | . 3561 | ND: | | 67 | | 24.572 | -3.387 | 81.545 | 1.00 23.80 |
| ATOM | 3562 | C | ASN B | 67 | | 26.982 | 0.401 | 83.513 | 1.00 25.34 |
| ATOM | 3563 | 0 | ASN B | 67 | | 26.524 | 1.539 | 83.448 | 1.00 22.53 |
| MOTA | 3564 3565 | N CA | THR B | 68 | | 27.664 | -0.031 | 84.568 | 1.00 23.65 |
| ATOM ATOM | 3566 | CB | THR B | 68 | | 27.903 | 0.863 | 85.696 | 1.00 25.25 |
| MOTA | 3567 | OG1 | | 68 68 | | 28.516 | 0.119 | 86.891 | 1.00 29.08 |
| ATOM | 3568 | CG2 | | 68 | | 27.561 | -0.826 | 87.396 | 1.00 25.94 |
| ATOM | 3569 | c | THR B | 68 | | 28.894 28.818 | 1.100 2.009 | 88.002 | 1.00 22.90 |
| ATOM | 3570 | O | THR B | 68 | | 28.576 | 3.156 | 85.287 | 1.00 25.91 |
| MOTA | 3571 | N | LEU B | 69 | | 29.861 | 1.702 | 85.661 84.519 | 1.00 28.47 |
| MOTA | 3572 | CA | LEU B | 69 | | 30.788 | 2.729 | 84.054 | 1.00 25.13 |
| MOTA | 3573 | CB | LEU B | 69 | | 31.915 | 2.122 | 83.201 | 1.00 24.37 |
| MOTA | 3574 | CG | LEU B | 69 | | 32.960 | 1.231 | 83.889 | 1.00 22.33 |
| ATOM | 3575 | CD1 | LEU B | 69 | | 34.006 | 0.786 | 82.859 | 1.00 22.57 |
| MOTA | 3576 | | LEU B | 69 | | 33.643 | 2.000 | | 1.00 23.20 |
| MOTA | 3577 | С | LEU B | 69 | | 30.036 | 3.764 | 83.229 | 1.00 23.02 |
| MOTA | 3578 | 0 | LEU B | 69 | | 30.190 | 4.966 | 83.444 | 1.00 18.98 |
| MOTA | 3579 | N | MET B | 70 | | 29.218 | 3.290 | 82.294 | 1.00 19.62 |
| ATOM | 3580 | CA | MET B | 70 | | 28.449 | 4.181 | 81.434 | 1.00 25.87 |
| ATOM | 3581 | CB | MET B | 70 | | 27.660 | 3.371 | 80.401 | 1.00 24.80 |
| MOTA | 3582 | CG | MET B | 70 | | 28.531 | 2.511 | 79.490 | 1.00 30.37 |
| TOM | 3583 | SD | MET B | 70 | | 27.592 | 1.599 | 78.227 | 1.00 30.35 |
| MOTA | 3584 | CE | MET B | 70 | | 26.922 | 2.986 | 77.245 | 1.00 30.20 |
| TOM | 3585 3586 | C | MET B | 70 70 | | 27.489 | 5.062 | 82.242 | 1.00 28.82 |
| MOTA | 3587 | O N | MET B | 70 71 | | 27.391 | 6.273 | 82.009 | 1.00 24.09 |
| MOT | 220/ | IA | GLU B | 71 | | 26.786 | 4.458 | 83.194 | 1.00 28.21 |

| MOTA | 3588 | B CA | GLI | U B | 71 | 25.837 | 5.207 | 84.008 | 1.00 27.4 | 5 |
|--------------|--------------|---------|-------------|-----|----------|------------------|------------------|------------------|--------------------------|--------|
| MOTA | 3589 | CE | GLI | U B | 71 | 25.014 | 4.268 | 84.889 | 1.00 30.7 | |
| ATOM | 3590 | CG | GL | UB | 71 | 24.072 | 5.005 | 85.832 | 1.00 33.6 | |
| MOTA | 3591 | | | U B | 71 | 23.044 | 5.867 | 85.096 | 1.00 37.5 | 1 |
| ATOM | 3592 | | :1 GL | | 71 | 22.333 | 6.638 | 85.773 | 1.00 35.4 | 7 |
| ATOM | 3593 | | | JB | 71 | 22.934 | 5.769 | 83.849 | 1.00 31.0 | |
| MOTA | 3594 | | | JВ | 71 | 26.559 | 6.209 | 84.887 | 1.00 29.1 | |
| MOTA | 3595 | | | J B | 71 | 26.115 | 7.341 | 85.035 | 1.00 23.9 | 6 |
| MOTA | 3596 | | | A B | | 27.671 | 5.781 | 85.481 | 1.00 27.7 | |
| ATOM | 3597 | | | | 72 | 28.454 | 6.662 | 86.340 | 1.00 27.5 | |
| MOTA | 3598 | | | | 72 | 29.663 | 5.920 | 86.909 | 1.00 23.2 | _ |
| ATOM | 3599 | | AL/ | | 72 | 28.924 | 7.886 | 85.563 | 1.00 28.0 | |
| ATOM | 3600 3601 | | AL.F GLU | | 72 73 | 28.895 | 8.999 | 86.079 | 1.00 23.2 | |
| ATOM | 3602 | | | | 73 | 29.356 29.846 | 7.684 | 84.322 | 1.00 26.4 | |
| MOTA MOTA | 3603 | | | | 73 | 30.658 | 8.801 | 83.529 | 1.00 29.0 | |
| ATOM | 3604 | | GLU | | 73 | 31.162 | 8.314 9.466 | 82.325 | 1.00 29.4 | |
| ATOM | 3605 | | | | 73 | 31.938 | 9.009 | 81.443 80.216 | 1.00 31.0 1.00 34.3 | |
| ATOM | 3606 | | | | 73 | 33.059 | 8.461 | 80.356 | 1.00 28.4 | |
| MOTA | 3607 | | | | 73 | 31.419 | 9.203 | 79.100 | 1.00 30.5 | |
| MOTA | 3608 | | GLU | | 73 | 28.744 | 9.734 | 83.045 | 1.00 31.9 | |
| ATOM | 3609 | | GLU | | 73 | 28.894 | 10.951 | 83.104 | 1.00 35.6 | |
| ATOM | 3610 | N | ARG | | 74 | 27.633 | 9.186 | 82.570 | 1.00 33.5 | |
| ATOM | 3611 | CA | ARG | В | 74 | 26.583 | 10.067 | 82.081 | 1.00 38.6 | |
| MOTA | 3612 | CB | ARG | В | 74 | 25.456 | 9.280 | 81.403 | 1.00 39.9 | |
| ATOM | 3613 | CG | ARG | В | 74 | 24.448 | 8.706 | 82.363 | 1.00 46.6 | 7 |
| MOTA | 3614 | CD | ARG | | 74 | 23.174 | 8.311 | 81.646 | 1.00 47.5 | 3 |
| MOTA | 3615 | NE | ARG | | 74 | 22.076 | 8.153 | .82.594 | 1.00 55.5 | 8 |
| ATOM | 3616 | CZ | ARG | | 74 | 21.609 | 9.136 | 83.362 | 1.00 56.0 | |
| MOTA | 3617 | | ARG | | 74 | 22.142 | 10.351 | 83.297 | 1.00 58.9 | |
| MOTA | 3618 | | ARG | | 74 | 20.601 | 8.910 | 84.192 | 1.00 53.6 | |
| ATOM | 3619 3620 | C O | ARG ARG | | 74 74 | 26.008 | 10.914 | 83.222 | 1.00 35.8 | |
| MOTA | 3621 | N | SER | | 75 | 25.778 25.794 | 12.107 | 83.048 | 1.00 29.4 | |
| MOTA MOTA | 3622 | CA | SER | | 75 | 25.794 | 10.302 11.014 | 84.386 85.539 | 1.00 31.0 | |
| ATOM | 3623 | СВ | SER | | 75 | 24.592 | 10.038 | 86.510 | 1.00 34.4 | |
| ATOM | 3624 | OG | SER | | 75 | 25.581 | 9.228 | 87.123 | 1.00 34.3 | |
| ATOM | 3625 | c | SER | | 75 | 26.339 | 11.754 | 86.288 | 1.00 35.4 | |
| ATOM | 3626 | 0 | SER | | 75 | 26.060 | 12.555 | 87.180 | 1.00 33.4 | |
| ATOM | 3627 | N | GLN | В | 76 | 27.584 | 11.473 | 85.922 | 1.00 33.2 | |
| ATOM | 3628 | CA | GLN | В | 76 | 28.739 | 12.082 | 86.565 | 1.00 35.6 | |
| ATOM | 3629 | CB | GLN | В | 76 | 28.818 | 13.572 | 86.241 | 1.00 30.13 | 1 |
| ATOM | 3630 | CG | GLN | В | 76 | 30.216 | 14.112 | 86.390 | 1.00 39.13 | 3 |
| ATOM | 3631 | CD | GLN | | 76 | 31.124 | 13.681 | 85.248 | 1.00 33.5 | 4 |
| MOTA | 3632 | OE1 | | | 76 | 31.052 | 12.546 | 84.761 | 1.00 29.2 | |
| MOTA | 3633 | NE2 | | | 76 | 31.995 | 14 583 | 84.827 | 1.00 40.93 | |
| ATOM | 3634 | C | GLN | | 76 | 28.624 | 11 892 | 88.079 | 1.00 37.88 | |
| MOTA | 3635 | 0 | GLN | | 76 | 28.901 | 12 908 | 88.858 | 1.00 32.74 | |
| ATOM | 3636 | N | SER | | 77 | 28.209 | 10.697 | 88.488 | 1.00 34.7 | |
| MOTA | 3637 | CA | SER | | 77 77 | 28.047 | 10.382 | 89.901 | 1.00 37.07 | |
| MOTA | 3638 | CB | SER | | 77 | 26.635 | 10.738 | 90.371 89.688 | 1.00 39.61 1.00 39.03 | 7 |
| ATOM | 3639 3640 | OG C | SER SER | | 77 | 25.678 28.265 | 9.941 8.897 | 90.112 | 1.00 35.99 | • |
| MOTA | 3641 | ò | SER | | 77 | 28.177 | 8.108 | 89.173 | 1.00 36.60 | |
| ATOM | 3642 | N | VAL | | 78 | 28.528 | 8.518 | 91.355 | 1.00 33.03 | , 1 |
| MOTA MOTA | 3643 | CA | VAL | | 78 | 28.753 | 7.124 | 91.685 | 1.00 33,41 | |
| MOTA | 3644 | CB | VAL | | 78 | 29.742 | 6.979 | 92.848 | 1.00 36.93 | |
| ATOM | 3645 | | VAL | | 78 | 29.955 | 5.499 | 93.163 | 1.00 34.37 | |
| MOTA | 3646 | | VAL | | 78 | 31.055 | 7.658 | 92.496 | 1.00 34.19 | |
| ATOM | 3647 | c | VAL | | 78 | 27.461 | 6.431 | 92.082 | 1.00 34.93 | 3 |
| ATOM | 3648 | o | VAL | | 78 | 26.897 | 6.703 | 93.143 | 1.00 28.25 | |
| ATOM | 3649 | N | PRO | В | 79 | 26.971 | 5.521 | 91.228 | 1.00 36.73 | 3 |
| ATOM | 3650 | CD | PRO | | 79 | 27.532 | 5.114 | 89.930 | 1.00 37.44 | l |
| ATOM | 3651 | CA | PRO | | 79 | 25.738 | 4.779 | 91.493 | 1.00 38.33 | |
| MOTA | 3652 | CB | PRO | | 79 | 25.668 | 3.826 | 90.301 | 1.00 38.68 | š |
| ATOM | 3653 | CG | PRO | В | 79 | 26.293 | 4.664 | 89.201 | 1.00 37.41 | |
| | | | | | | | | | | |

| 3 00 3 | 205 | 4 0 | 220 | | | | | | |
|--------------|--------------|------|-------|------|-------------|----------|---------|------|-------|
| ATOM | | | | | 25.788 | 3 4.046 | 92.834 | 1.00 | 36.92 |
| MOTA | | | PRO | B 79 | 26.854 | 3.648 | 93.298 | 1.00 | 33.03 |
| MOTA | 1 365 | 6 N | LYS | B 80 | 24.623 | 3 .881 | | | 38.43 |
| ATOM | 365 | 7 C | A LYS | | 24.482 | | | 1.00 | 30.43 |
| ATOM | | | | | | | | 1.00 | 39.73 |
| | | | | | 23.003 | | | | 43.33 |
| ATOM | | | | | 22.679 | 2:129 | 96.262 | 1.00 | 44.60 |
| MOTA | 366 | o ci | D LYS | B 80 | 21.198 | 1.742 | 96.287 | | 48.09 |
| ATOM | 366 | 1 C | E LYS | B 80 | 20.805 | | | | |
| MOTA | | | | | | | | | 50.12 |
| | | | | | 20.932 | 1.890 | | | 53.16 |
| ATOM | | | LYS | | 25.315 | | 94.854 | 1.00 | 40.35 |
| MOTA | 366 | 4 0 | LYS | B 80 | - 25.181 | 1.011 | 94.047 | 1.00 | 36.67 |
| MOTA | 366 | 5 N | GLY | B 81 | 26.173 | 1.880 | | 1 00 | 38.26 |
| ATOM | | б СА | | | 26.996 | | | | |
| | | | GLY | | | | | | 34.69 |
| ATOM | | | | | 28.066 | | | | 34.63 |
| MOTA | | | GLY : | | 28.861 | -0.513 | 95.255 | 1.00 | 33.92 |
| MOTA | 3669 | э и | ALA : | B 82 | 28.100 | 1.178 | 93.992- | | 31.26 |
| ATOM | 3670 | CA | ALA : | B 82 | . 29.082 | | 92.936 | | 34.88 |
| ATOM | 3671 | | | | 28.755 | | | 1.00 | 34.88 |
| | | | | | | | 91.751 | | 23.13 |
| MOTA | 3672 | | ALA : | | 30.517 | | 93.405 | 1.00 | 36.85 |
| MOTA | 3673 | 3 0 | ALA 1 | B 82 | 31.461 | 0.580 | 92.945 | 1.00 | 32.17 |
| ATOM | 3674 | N | ARG 1 | B 83 | 30.677 | 2.168 | 94.323 | | 36.52 |
| ATOM | 3675 | CA | | | 31.994 | 2.522 | 94.830 | | |
| | 3676 | | ARG I | | | | | | 38.75 |
| ATOM | | | | | 31.865 | 3.616 | 95.885 | | 40.24 |
| MOTA | 3677 | | ARG I | | 33.187 | 4.180 | 96.330 | 1.00 | 49.12 |
| MOTA | 3678 | CD | ARG E | 83 | 33.015 | 5.239 | 97.404 | | 53.26 |
| ATOM | 3679 | NE | ARG E | 83 | 34.240 | 6.010 | 97.624 | | 59.30 |
| ATOM | 3680 | CZ | ARG E | | 35.437 | 5.486 | | | |
| ATOM | 3681 | | | | | | 97.883 | | 61.56 |
| | | | | | 35.598 | 4.170 | 97.958 | | 63.53 |
| ATOM | 3682 | | | | 36.479 | 6.285 | 98.073 | 1.00 | 62.02 |
| ATOM - | 3683 | С | ARG E | 83 | 32.719 | 1.326 | 95.426 | | 37.75 |
| ATOM | 3684 | 0 | ARG B | 83 | 33.893 | 1.094 | 95.146 | | 37.18 |
| ATOM | 3685 | N | GLU B | | 32.011 | 0.564 | | 1.00 | 37.10 |
| ATOM | 3686 | CA | GLU B | | | | 96.249 | 1.00 | 35.29 |
| | | | | | 32.581 | -0.609 | 96.898 | | 35.29 |
| ATOM | 3687 | CB | GLU B | | 31.876 | -0.855 | 98.236 | 1.00 | 40.14 |
| MOTA | 3688 | CG | GLU B | 84 | 30.443 | -0.383 | 98.240 | | 46.30 |
| ATOM | 3689 | CD | GLU B | 84 | 30.356 | 1.132 | 98.293 | | 48.30 |
| MOTA | 3690 | OE1 | GLU B | | 29.339 | 1.690 | 97.834 | | 43.07 |
| ATOM | 3691 | OE2 | | 84 | | | | | |
| | | | | | 31.306 | 1.762 | 98.814 | | 50.07 |
| ATOM | 3692 | C | GLU B | 84 | 32.527 | -1.880 | 96.055 | 1.00 | 32.90 |
| MOTA | 3693 | 0 | GLU B | 84 | 33.371 | -2.765 | 96.193 | 1.00 | 28.68 |
| MOTA | 3694 | Ν. | LYS B | 85 | 31.533 | -1.984 | 95.187 | 1.00 | 27.12 |
| ATOM | 3695 | CA | LYS B | 85 | 31.412 | -3.177 | 94.361 | | 30.46 |
| ATOM | 3696 | CB | LYS B | 85 | 29.950 | | | | |
| | | | | | | -3.401 | 93.967 | | 30.01 |
| ATOM | 3697 | CG | LYS B | 85 | 29.717 | -4.643 | 93.117 | | 28.40 |
| ATOM | 3698 | CD | LYS B | 85 | 28.234 | -4.807 | 92.775 | 1.00 | 32.87 |
| A. OM | 3699 | CE | LYS B | 85. | 28.000 | -6.048 | 91.928 | | 34.15 |
| A. OM | 3700 | NZ | LYS B | 85 | 26.582 | -6:186 | 91.507 | | 35.34 |
| MOLA | 3701 | C | LYS B | 85 | 32.267 | | | | |
| | 3702 | | | | | -3.096 | 93.101 | | 28.98 |
| ATOM | - | 0 | LYS B | 85 | 32.817 | -4.098 | 92.652 | | 24.69 |
| ATOM | 3703 | N | TYR B | 86 | 32.391 | -1.896 | 92.550 | 1.00 | 27.81 |
| ATOM | 3704 | CA | TYR B | 86 | 33.141 | -1.692 | 91.319 | 1.00 | 27.56 |
| ATOM | 3705 | CB | TYR B | 86 | 32.206 | -1.050 | 90.288 | | 28.88 |
| ATOM · | 3706 | CG | TYR B | 86 | 31.008 | | | | |
| | | | | | | -1.927 | 89.951 | | 31.29 |
| MOTA | 3707 | CD1 | TYR B | 86 | 31.178 | -3.137 · | 89.276 | 1.00 | 26.99 |
| MOT A | 3708 | CE1 | TYR B | 86 | 30.095 | -3.955 | 88.965 | 1.00 | 26.97 |
| MOTA | 370 <i>9</i> | CD2 | TYR B | 86 | 29.713 | -1.553 | 90.315 | | 28.38 |
| ATOM | 3710 | CE2 | TYR B | 86 | 28.611 | -2.370 | 90.008 | 1.00 | |
| ATOM | 3711 | CZ | TYR B | 86 | 28.815 | • | | | |
| | | | | | | -3.569 | 89.331 | 1.00 | |
| ATOM | 3712 | OH | TYR B | 86 | 27.747 | -4.379 | 89.008 | 1.00 | 22.70 |
| MOTA | 3713 | C | TYR B | 86 | 34.422 | -0.870 | 91.489 | 1.00 | 24.64 |
| ATOM | 3714 | 0 | TYR B | 86 | 35.160 | -0.645 | 90.530 | 1.00 | |
| ATOM | 3715 | | ASN B | 87 | 34.674 | -0.418 | 92.711 | 1.00 | |
| | 3716 | | | | | | | | |
| MOTA | | | ASN B | 87 | 35.881 | 0.341 | 93.032 | 1.00 | |
| ATOM | 3717 | | ASN B | 87 | 37.105 | -0.561 | 92.866 | 1.00 | 28.92 |
| ATOM | 3718 | CG . | asn B | 87 | 38.343 | 0.019 | 93.506 | 1.00 | |
| ATOM | 3719 | OD1 | ASN B | 87 | 38.309 | 0.452 | 94.659 | 1.00 | |
| 112 011 | | | | | | 0.352 | | | |

| MOTA | 3720 | ND2 | ASN | В | 87 | 39.449 | 0.012 | 92.775 | 1.00 35.86 |
|-------|---------------|-----|------------|----|------|----------------|--------|---------|------------|
| | | | | | | | 1.622 | 92.223 | 1.00 29.72 |
| ATOM | 3721 | С | ASN | B | 87 | 36.070 | | | |
| MOTA | 3722 | 0 | ASN | В | 87 | 37.194 | 1.998 | 91.876 | 1.00 24.01 |
| | | | | | | 34.956 | 2.282 | 91.932 | 1.00 29.43 |
| MOTA | 3723 | N | ILE | | 88 | | | | • |
| MOTA | 3724 | CA | ILE | В | 88 | 34.945 | 3.536 | 91.196 | 1.00 30.64 |
| | 3725 | CB | ILE | | 88 | 33.959 | 3.464 | 90.027 | 1.00 37.12 |
| ATOM- | | | | | | | | 00.02. | |
| ATOM | 3726 | CG2 | ILE | В | 88 | 33.821 | 4.829 | 89.379 | 1:00 40.62 |
| | 3727 | CG1 | ILE | R | 88 | 34.421 | 2.433 | 89.008 | 1.00 35.43 |
| MOTA | | | | | | | | | |
| MOTA | 3728 | CD1 | ILE | В | 88 | 35.684 | 2.821 | 88.324 | 1.00 41.80 |
| ATOM | 3729 | С | ILE | В | 88 | 34.483 | 4.669 | 92.118 | 1.00 31.90 |
| | | | | | | 33.681 | 4.445 | 93.024 | 1.00 28.86 |
| MOTA | 3730 | 0 | ILE | | 88 | | | | |
| MOTA | 3731 | N | GLY | В. | 89 | 34.977 | 5.881 | 91.875 | 1.00 30.36 |
| | 3732 | CA | GLY | D | 89 - | 34.574 | 7.022 | 92.686 | 1.00 29.54 |
| ATOM | | | | | | | | | |
| ATOM | 3733 | С | GLY | В | 89 | 35.601 | 7.524 | 93.685 | 1.00 31.49 |
| ATOM | 3734 | 0 | GLY | R | 89 | 35.497 | 8.652 | 94.177 | 1.00 37.26 |
| | | | | | | | 6.687 | 94.005 | 1.00 30.97 |
| ATOM | 3735 | N | GLY | | 90 | 36.583 | | | |
| ATOM | 3 7 36 | CA | GLY | В | 90 | 37.612 | 7.086 | 94.949 | 1.00 31.03 |
| | | | GLY | | 90 | 38.655 | 7.936 | 94.247 | 1.00 34.78 |
| MOTA | 3737 | С | | | | | | | |
| ATOM | 3738 | 0 | GLY | В | 90 | 38.455 | 8.344 | 93.103 | 1.00 32.73 |
| ATOM | 3739 | N | TYR | В | 91 | 39.772 | 8.201 | 94.915 | 1.00 29.39 |
| | | | | | | 40.820 | 9.023 | 94.322 | 1.00 28.15 |
| ATOM | 3740 | CA | TYR | В | 91 | | | | |
| ATOM | 3741 | CB | TYR | В | 91 | 41.810 | 9.463 | 95.405 | 1.00 27.29 |
| | | CG | TYR | | 91 | 42.609 | 8.330 | 96.007 | 1.00 26.60 |
| MOTA | 3742 | | | | | | | | |
| MOTA | 3743 | CD1 | TYR | В | 91 | 43.738 | 7.823 | 95.359 | 1.00 28.55 |
| ATOM | 3744 | CE1 | TYR | В | 91 | 44.456 | 6.762 | 95.896 | 1.00 28.75 |
| | | | | | | 42.219 | 7.741 | 97.208 | 1.00 28.35 |
| ATOM | 3745 | CD2 | TYR | | 91 | | | | |
| MOTA | 3746 | CE2 | ŤΥR | В | 91 | 42.927 | 6.680 | 97.751 | 1.00 27.58 |
| | 3747 | CZ | TYR | R | 91 | 44.043 | 6.196 | 97.094 | 1.00 30.12 |
| MOTA | | | | | | 44.753 | 5.154 | 97.637 | 1.00 36.59 |
| ATOM | 3748 | OH | TYR | | 91 | | | | |
| ATOM | 3749 | С | TYR | В | 91 | 41.563 | 8.271 | 93.226 | 1.00 29.27 |
| ATOM | 3750 | 0 | TYR | В | 91 | 42.109 | 8.874 | 92.308 | 1.00 25.22 |
| | | | | | 92 | 41.568 | 6.948 | 93.318 | 1.00 28.32 |
| MOTA | 3 751 | N | GLU | | | | | | |
| ATOM | 3752 | CA | GLU | В | 92 | 42.286 | 6.124 | 92.350 | 1.00 27.06 |
| ATOM | 3753 | CB | GLU | В | 92 | 42.474 | 4.726 | 92.924 | 1.00 23.35 |
| | | | | | 92 | 43.502 | 3.884 | 92.221 | 1.00 29.80 |
| ATOM | 3754 | CG | GLU | | | | | | 1.00 35.34 |
| ATOM | 3755 | CD | ${	t GLU}$ | В | 92 | 43.585 | 2.500 | 92.826 | |
| ATOM | 3756 | OE1 | GLU | В | 92 | 42.742 | 1.645 | 92.477 | 1.00 32.15 |
| | | OE2 | GLU | | 92 | 44.475 | 2.278 | 93.678 | 1.00 31.61 |
| ATOM | 3757 | | | | | | | | |
| ATOM | 3758 | С | GLU | В | 92 | 41.594 | 6.024 | 90.997 | 1.00 23.42 |
| MOTA | 3759 | 0 | GLU | В | 92 | 42.204 | 6.260 | 89.962 | 1.00 20.47 |
| | | | ASN | | 93 | 40.314 | 5.677 | 91.017 | 1.00 18.85 |
| MOTA | 3760 | N | | | | | | | |
| ATOM | 3 761 | CA | ASN | В | 93 | 39.534 | 5.509 | 89.795 | 1.00 21.96 |
| ATOM | 3762 | CB | ASN | В | 93 | 39.165 | 4.033 | 89.664 | 1.00 23.90 |
| | | | | | 93 | 40.351 | 3.120 | 89.943 | 1.00 24.78 |
| ATOM | 3763 | CG | ASN | | | | | | 1.00 22.35 |
| MOTA | 3764 | OD1 | ASN | В | 93 | 41.362 | 3.160 | 89.239 | |
| | 3765 | ND2 | ASN | В | 93 | 40.240 | 2.311 | 90.987 | 1.00 13.35 |
| ATOM | | | | | 93 | 38.285 | 6.362 | 89.944 | 1.00 25.16 |
| MOTA | 3766 | С | ASN | | | | | | |
| MOTA | 3767 | 0 | ASN | В | 93 | 37.183 | 5.843 | 90.121 | 1.00 20.91 |
| | 3768 | N | PRO | R | 94 | 38.449 | 7.693 | 89.887 | 1.00 26.37 |
| ATCM | | | | | | | 8.389 | 89.716 | 1.00 19.35 |
| MOTA | 3769 | CD | PRO | | 94 | 39.738 | | | |
| MOTA | 3770 | CA | PRO : | В | 94 | 37.3 73 | 8.676 | 90.024 | 1.00 24.59 |
| | 2772 | | PRO | | 94 | 38.147 | 9.972 | 90.200 | 1.00 25.95 |
| MOTA | 3771 | CB | | | | | | | |
| MOTA | 3772 | CG | PRO | В | 94 | 39.297 | 9.740 | 89.223 | 1.00 22.60 |
| | 3773 | С | PRO : | В | 94 | 36.384 | 8.777 | 88.873 | 1.00 28.74 |
| MOTA | | | PRO : | | 94 | 36.562 | 8.176 | 87.808 | 1.00 25.77 |
| MOTA | 3774 | 0 | | | | | | 89.112 | |
| MOTA | 3775 | N | VAL : | В | 95 | 35.332 | 9.553 | | 1.00 27.14 |
| | 3776 | CA | VAL : | В | 95 | 34.317 | 9.812 | 88.103 | 1.00 25.94 |
| MOTA | | | | | | | | 88.742 | 1.00 23.75 |
| ATOM | 3 <i>777</i> | CB | VAL | | 95 | 33.035 | 10.393 | | |
| ATOM | 3778 | CG1 | VAL : | В | 95 | 32.067 | 10.855 | 87.662 | 1.00 26.34 |
| | 3779 | CG2 | VAL : | | 95 | 32.376 | 9.346 | 89.622 | 27.59 |
| atom | | | | | | | | 87.175 | 1.00 25.69 |
| ATOM | 3780 | С | VAL | | 95 | 34.912 | 10.861 | | |
| ATOM | 3781 | 0 | VAL : | В | 95 | 35.564 | 11.793 | 87.641 | 1.00 25.25 |
| | - | N | SER | | 96 | 34.708 | 10.699 | 85.871 | 1.00 28.02 |
| ATOM | 3782 | | | | | | | 84.868 | 1.00 24.82 |
| MOTA | 3783 | CA | SER | | 96 | 35.199 | 11.647 | | |
| ATOM | 3784 | CB | SER | B | 96 | 36.729 | 11.705 | .84.850 | 1.00 25.90 |
| | 3785 | OG | SER | | 96 | 37.274 | 10.548 | 84.229 | 1.00 23.99 |
| ATOM | 1 7 0 - | ~~ | | - | | | | | |

| ATOM | 3786 | C | SER B | 96 | | 34.726 | 11.127 | 83.519 | 1.00 | 26.22 |
|------|------|-----|----------|-------------|---|--------|----------------|--------|------|-------|
| ATOM | 3787 | 0 | SER B | 96 | | 33,943 | 10.174 | 83.462 | 1.00 | 23.57 |
| ATOM | 3788 | N | TYR B | 97 | | 35.195 | 11.744 | 82.438 | | 22.83 |
| ATOM | 3789 | | | 97 | | 34.818 | 11.279 | 81.110 | | 28.59 |
| ATOM | 3790 | | _ | 97 | | 34.536 | 12.452 | 80.165 | | 31.45 |
| | 3791 | ĊG | | 97 | | 33.279 | | | | |
| ATOM | | | _ | | | | 13.203 | 80.548 | | 35.09 |
| ATOM | 3792 | CD | | 97 | | 33.316 | 14.239 | 81.480 | | 32.87 |
| ATOM | 3793 | CE | | 97 | | 32.148 | 14.863 | 81.911 | | 37.73 |
| ATOM | 3794 | CD | _ | 97 | | 32.036 | 12.812 | 80.049 | | 34.85 |
| ATOM | 3795 | CE | | 97 | | 30.858 | 13.430 | 80.475 | | 38.61 |
| ATOM | 3796 | CZ | | 97 | | 30.924 | 14.453 | 81.408 | 1.00 | 39.45 |
| ATOM | 3797 | OH | TYR B | 97 | | 29.768 | 15.047 | 81.852 | 1.00 | 35.36 |
| ATOM | 3798 | C. | TYR B | 97 | | 35.883 | 10.354 | 80.534 | 1.00 | 28.93 |
| ATOM | 3799 | 0 | TYR B | 97 | | 35.859 | 9.992 | 79.358 | 1.00 | 28.26 |
| ATOM | 3800 | N | ALA B | 98 | | 36.822 | 9.968 | 81.385 | | 29.09 |
| ATOM | 3801 | CA | ALA B | 98 | | 37.866 | 9.044 | 80.980 | | 26.88 |
| ATOM | 3802 | CB | ALA B | 98 | | 39.167 | 9.369 | 81.692 | | 27.99 |
| ATOM | 3803 | С | ALA B | 98 | | 37.395 | 7.657 | 81.382 | | 22.53 |
| ATOM | 3804 | Ō | ALA B | 98 | | 37.721 | 6.675 | 80.722 | | 21.98 |
| ATOM | 3805 | N | MET B | 99 | | 36,603 | 7.595 | 82.453 | | 23.51 |
| ATOM | 3806 | CA | MET B | 99 | | 36.106 | 6.326 | 82.986 | | 26.36 |
| | 3807 | СВ | MET B | 99 | | 35.179 | 6.568 | 84.185 | | 24.05 |
| ATOM | 3808 | CG | MET B | 99 | | | 7.188 | 83.875 | | |
| MOTA | | | MET B | | | 33.822 | | | 1.00 | |
| ATOM | 3809 | SD | | 99 | | 32.966 | 7.704 | 85.406 | | 27.91 |
| MOTA | 3810 | CE | MET B | 99 | | 33.106 | 6.227 | 86.409 | | 22.12 |
| ATOM | 3811 | C | MET B | 99 | | 35.430 | 5.435 | 81.953 | | 25.76 |
| ATOM | 3812 | 0 | MET B | 99 | | 35.544 | 4.212 | 82.031 | | 26.11 |
| ATOM | 3813 | N | | 100 | | 34.724 | 6.027 | 80.992 | | 22.17 |
| ATOM | 3814 | CA | | 100 | | 34.107 | 5.222 | 79.940 | | 22.35 |
| ATOM | 3815 | CB | | 100 | | 32.582 | 5.133 | 80.088 | | 22.01 |
| MOTA | 3816 | CG | | 100 | | 31.947 | 4.254 | 79.038 | | 24.22 |
| MOTA | 3817 | | | 10 0 | | 32.143 | 2.872 | 79.061 | | 26.61 |
| MOTA | 3818 | | | 100 | | 31.280 | 4.813 | 77.953 | | 21.22 |
| ATOM | 3819 | CE1 | PHE B 1 | 00 | | 31.691 | 2.059 | 78.012 | 1.00 | 26.91 |
| ATOM | 3820 | CE2 | PHE B | 100 | | 30.825 | 4.010 | 76.894 | 1.00 | 24.80 |
| ATOM | 3821 | cz | PHE B 1 | 100 | | 31.033 | 2.632 | 76.924 | 1.00 | 24.85 |
| ATOM | 3822 | С | PHE B 1 | .00 | 3 | 34.425 | 5.695 | 78.514 | 1.00 | 24.86 |
| MOTA | 3823 | 0 | PHE B 1 | .00 | 3 | 34.922 | 4.920 | 77.694 | 1.00 | 21.40 |
| MOTA | 3824 | N | THR B 1 | .01 | | 34.131 | 6.957 | 78.204 | 1.00 | 24.24 |
| ATOM | 3825 | CA | THR B 1 | .01 | 3 | 34.390 | 7.469 | 76.854 | 1.00 | 24.54 |
| ATOM | 3826 | CB | THR B 1 | .01 | 3 | 33.914 | 8.926 | 76.708 | 1.00 | 24.46 |
| ATOM | 3827 | 0G1 | THR B 1 | 01 | 3 | 32.504 | 8.985 | 76.953 | | 27.64 |
| MOTA | 3828 | CG2 | THR B 1 | 01 | 3 | 34.191 | 9.445 | 75.297 | 1.00 | 22.19 |
| ATOM | 3829 | С | THR B 1 | | | 35.872 | 7.387 | 76.483 | | 25.26 |
| ATOM | 3830 | 0 | THR B 1 | | | 6.231 | 6.856 | 75.430 | | 25.47 |
| ATOM | 3831 | N | GLY B 1 | | | 6.725 | 7.916 | 77.350 | | 23.74 |
| ATOM | 3832 | CA | | 02 | | 8.153 | 7.867 | 77.096 | | 24.53 |
| ATOM | 3833 | C | | 02 | | 8.657 | 6.434 | 77.046 | | 24.06 |
| ATOM | 3834 | ō | GLY B 1 | | | 9.346 | 6.045 | 76.100 | | 22.53 |
| ATOM | 3835 | N | SER B 1 | | | 8.316 | 5.651 | 78.067 | | 22.02 |
| | | CA | SER B 1 | | | 8.730 | | 78.146 | 1 00 | 20.45 |
| ATOM | 3836 | | SER B 1 | | 2 | 8.193 | 4.253 3.613 | 79.427 | | |
| ATOM | 3837 | CB | | | | | | | | 25.21 |
| ATOM | 3838 | OG | SER B 1 | | | 8.820 | 4.166 | 80.567 | | 26.48 |
| MOTA | 3839 | C | SER B 1 | | | 8.268 | 3.446 | 76.938 | | 20.53 |
| MOTA | 3840 | 0 | SER B 1 | | | 9.034 | 2.669 | 76.372 | | 16.82 |
| MOTA | 3841 | N | SER B 1 | | | 7.014 | 3.642 | 76.542 | | 17.11 |
| MOTA | 3842 | CA | SER B 1 | | | 6.462 | 2.937 | 75.395 | | 23.32 |
| ATOM | 3843 | CB | SER B 1 | | | 4.980 | 3.289 | 75.228 | | 22.93 |
| ATOM | 3844 | OG | SER B 1 | | | 4.424 | 2.557 | 74.161 | | 24.75 |
| MOTA | 3845 | С | SER B 1 | 04 | 3 | 7.221 | 3.288 | 74.116 | | 21.97 |
| ATOM | 3846 | 0 | SER B 1 | | | 7.451 | 2.434 | 73.256 | 1.00 | 22.83 |
| MOTA | 3847 | N | LEU B 1 | 05 | 3 | 7.619 | 4.549 | 73.997 | | 23.00 |
| ATOM | 3848 | CA | LEU B 10 | 25 | 3 | 8.354 | 5.007 | 72.825 | 1.00 | 25.12 |
| ATOM | 3849 | CB | LEU B 10 | 75 | 3 | 8.443 | 6.536 | 72.859 | 1.00 | 29.25 |
| MOTA | 3850 | CG | LEU B 10 | 75 | | 8.702 | 7.289 | 71.553 | 1.00 | 34.27 |
| ATOM | 3851 | CD1 | LEU B 1 | 05 | | 7.662 | 6.888 | 70.512 | 1.00 | 31.51 |
| | | | | | | | | | | |

| ATOM | 3852 | CD2 | LEU | B 105 | | 38.629 | 8.802 | 71.819 | 1.00 | 34.30 |
|--------------|--------------|-------|-------|--------------------|---|------------------|------------------|------------------|------|----------------|
| ATOM | 3853 | С | LEU | B 105 | | 39.755 | 4.374 | 72.813 | | 27.39 |
| MOTA | 3854 | . 0 | | B 105 | | 40.262 | 3.955 | 71.765 | | 20.15 |
| ATOM | 3855 | N | ALA | B 106 | | 40.371 | 4.293 | 73.988 | | 23.62 |
| ATOM | 3856 | CA | ALA | B 106 | | 41.704 | 3.692 | 74.115 | | 22.73 |
| ATOM | 3857 | СВ | ALA | B 106 | | 42.263 | 3.939 | 75.529 | | 17.46 |
| ATOM | 3858 | | | B 106 | | 41.639 | 2.189 | 73.846 | 1.00 | 22.77 |
| ATOM | 3859 | | ALA | B 106 | | 42.583 | 1.597 | 73.316 | | 24.98 |
| ATOM | | | THR | | | 40.523 | 1.567 | 74.224 | | 23.54 |
| ATOM | 3861 | | THR | | | 40.355 | 0.132 | 74.033 | | 19.76 |
| MOTA | 3862 | | THR | | | 39.236 | -0.410 | 74.947 | | 22.85 |
| ATOM | 3863 | | THR | B 107 | | 39.572 | -0.128 | 76.306 | | 16.29 |
| ATOM | 3864 | CG2 | THR | B 107 | | 39.085 | -1.917 | 74.787 | | 17.21 |
| ATOM | 3865 | С | THR | B 107 | | 40.036 | -0.169 | 72.571 | | 23.47 |
| ATOM | 3866 | 0 | THR | B 107 | | 40.540 | -1.138 | 72.001 | | 19.25 |
| ATOM | 3867 | N | GLY | B 108 | | 39.191 | 0.656 | 71.959 | | 24.87 |
| ATOM | 3868 | CA | GLY | B 108 | | 38.879 | 0.434 | 70.560 | | 21.32 |
| MOTA | 3869 | С | GLY | B 108 | | 40.161 | 0.594 | 69.757 | | 22.01 |
| ATOM | 3870 | 0 | GLY | B 108 | | 40.388 | -0.099 | 68.761 | 1.00 | 20.46 |
| MOTA | 3871 | N | SER | B 109 | | 41.018 | 1.508 | 70.197 | | 19.89 |
| MOTA | 3872 | CA | SER | B 109 | | 42.274 | 1.749 | 69.499 | 1.00 | 19.37 |
| MOTA | 3873 | CB | SER | B 109 | | 42.993 | 2.956 | 70.107 | 1.00 | 18.28 |
| MOTA | 3874 | OG | SER | в 109 | | 42.250 | 4.145 | 69.882 | | 21.29 |
| MOTA | 3875 | С | SER | B 109 | | 43.168 | 0.513 | 69.542 | 1.00 | 20.70 |
| ATOM | 3876 | 0 | SER | | | 43.940 | 0.261 | 68.617 | 1.00 | 20.69 |
| MOTA | 3877 | N | THR | | | 43.065 | -0.259 | 70.616 | | 20.54 |
| ATOM | 3878 | CA | THR | | | 43.858 | -1.475 | 70.729 | | 19.98 |
| ATOM | 3879 | CB | THR | | • | 43.826 | -2.043 | 72.158 | | 20.63 |
| ATOM | 3880 | | THR | | | 44.632 | -1.215 | 73.007 | | 20.72 |
| MOTA | 3881 | | THR | | | 44.371 | -3.470 | 72.188 | | 20.05 |
| ATOM | 3882 | | THR | | | 43.333 | -2.507 | 69.738 | | 21.61 |
| MOTA | 3883 | | THR : | | | 44.115 | -3.239 | 69.127 | | 18.11 |
| ATOM | 3884 | | VAL : | | | 42.012 | -2.557 | 69.567 | | 18.29 |
| ATOM | 3885 | | | B _. 111 | | 41.432 | -3:486 | 68.608 | | 20.36 |
| ATOM | 3886 3887 | | VAL I | B 111 B 111 | | 39.886 39.324 | -3.494 | 68.677 | | 23.94 |
| MOTA | 3888 | | VAL I | | | 39.426 | -4.442 -3.937 | 67.619 70.063 | | 24.37 21.50 |
| MOTA MOTA | 3889 | | VAL I | | | 41.872 | -3.937 | 67.197 | | 20.35 |
| ATOM | 3890 | | | 3 111 | | 42.146 | -3.936 | 66.362 | | 23.29 |
| ATOM . | 3891 | | | 3 112 | | 41.953 | -1.775 | 66.937 | | 22.07 |
| ATOM | 3892 | | GLN I | | | 42.367 | -1.290 | 65.617 | | 22.34 |
| ATOM | 3893 | | GLN I | | | 42.199 | 0.230 | 65.513 | | 24.54 |
| ATOM | 3894 | | GLN I | | | 40.810 | 0.729 | 65.843 | | 20.63 |
| ATOM | 3895 | CD (| GLN E | 3 112 | | 40.700 | 2.236 | 65.742 | | 21.19 |
| MOTA | 3896 | OE1 (| GLN E | 3 112 | | 40.664 | 2.794 | 64.645 | | 26.73 |
| ATOM | 3897 | NE2 | GLN E | 3 112 | | 40.667 | 2.905 | 66.886 | 1.00 | 18.73 |
| ATCM | 3898 | c (| GLN E | 3 112 | | 43.826 | -1.635 | 65.363 | | 23. 1 |
| ATOM | 389 9 | 0 (| GLN E | 3 112 | | 44.195 | -2.020 | 64.257 | | 15.79 |
| MOTA | 390 0 | N i | ALA E | 113 | | 44.660 | -1.476 | 66.389 | 1.00 | 20.60 |
| ATOM | 3901 | | ALA E | | | 46.070 | -1.790 | 66.249 | 1.00 | 18.02 |
| MOTA | 3902 | | ALA E | | | 46.794 | -1.536 | 67.548 | 1.00 | 20.84 |
| ATOM | 3903 | | ALA E | | | 46.170 | -3.262 | 65.863 | | 23.78 |
| MOTA | 3904 | | ALA E | | | 46.982 | -3.642 | 65.023 | | 19.83 |
| ATOM | . 3905 | | ILE E | | | 45.331 | -4.091 | 66.477 | | 21.45 |
| ATOM | 3906 | | ILE E | | | 45.344 | -5.511 | 66.168 | | 24.26 |
| ATOM | 3907 | | ILE B | | | 44.507 | -6.306 | 67.191 | | 20.72 |
| MOTA | 3908 | | ILE B | | | 44.476 | -7.779 | 66.800 | | 21.92 |
| ATOM | 3909 | | LLE E | | | 45.116 | -6.144 | 68.593 | | 24.32 |
| ATOM | 3910 | | LE B | | | 44.364 | -6.872 | 69.694 | | 19.01 |
| ATOM | 3911 | | LE B | | | 44.808 | -5.765 | 54.753 | | 26.75 |
| ATOM | 3912 | | LE B | | | 45.305 | -6.640 | 64.032 | - | 20.18 |
| ATOM | 3913 | | LU B | | | 43.792 | -5.009 | 64.347 | | 24.69 |
| ATCM | 3914 | | LU B | | | 43.243 | -5.198 | 63.005 | | 29.26 |
| ATOM | 3915 | | LU B | | | 42.043 | -4.278 | 62.770 | | 29.07 |
| ATCM | 3916 | | LU B | | | 40.940 | -4.421 | 63.800 | | 32.31 |
| ATOM | 3917 | CD G | LU B | 110 | | 39.757 | -3.519 | 63.516 | 1.00 | 38.14 |
| | | | | | | | | | | |

| _ | | | | | | | | |
|------|-------|-----|---------|---------|--------|----------------|--------|------------|
| MOTA | 3918 | OE | 1 GLU | B 115 | 39.980 | -2.374 | 63.072 | 1.00 40.63 |
| ATOM | 3919 | | | | 38.607 | | | |
| | | | _ | | | | 63.758 | 1.00 39.86 |
| ATOM | 3920 | | | B 115 | 44.334 | | 61.974 | 1.00 31.52 |
| ATOM | 3921 | 0 | GLU I | B 115 | 44.444 | -5.603 | 60.964 | 1.00 26.43 |
| ATOM | 3922 | N | GLU I | 3 116 | 45.141 | | 62.234 | 1.00 26.04 |
| | | | | | | | | |
| MOTA | 3923 | | | | 46.226 | | 61.324 | 1.00 26.21 |
| ATOM | 392,4 | CB | GLU I | 3 116 | 46.909 | -2.227 | 61.775 | 1.00 23.21 |
| MOTA | 3925 | CG | GLU | 3 116 . | 46.055 | -0.983 | 61.601 | 1.00 23.82 |
| ATOM | 3926 | | | | | | | |
| | | CD | | | 45.576 | -0.817 | 60.163 | 1.00 31.43 |
| ATOM | 3927 | OE. | 1 GLU E | 3 116 | 46.425 | -0.734 | 59.253 | 1.00 26.45 |
| MOTA | 3928 | OE: | 2 GLU E | 3 116 . | 44.349 | -0.771 | 59.945 | 1.00 24.59 |
| ATOM | 3929 | C | GLU F | | 47.256 | | | |
| | | | | | | -4.644 | 61.243 | 1.00 28.60 |
| MOTA | 3930 | 0 | GLU E | | 47.857 | -4.884 | 60.189 | 1.00 25.01 |
| MOTA | 3931 | N | PHE F | 3 117 | 47.470 | -5.324 | 62.363 | 1.00 26.22 |
| ATOM | 3932 | CA | PHE F | 3 117 | 48.421 | -6.425 | 62.400 | 1.00 28.05 |
| ATOM | 3933 | СВ | PHE E | | | | | |
| | | | | | 48.516 | -7.007 | 63.805 | 1.00 32.15 |
| MOTA | 3934 | CĠ | PHE E | | 49.278 | -8.299 | 63.869 | 1.00 33.88 |
| MOTA | 3935 | CD: | l PHE E | 117 | 50.656 | -8.321 | 63.713 | 1.00 33.52 |
| ATOM | 3936 | CD | PHE E | : 117 | 48.604 | | 64.054 | 1.00 32.83 |
| | | | | | | | | |
| MOTA | 3937 | | PHE E | | 51.356 | -9.521 | 63.740 | 1.00 31.67 |
| MOTA | 3938 | CE | PHE B | 117 | 49.294 | -10.710 | 64.082 | 1.00 35.69 |
| MOTA | 3939 | CZ | PHE B | 117 | 50.674 | -10.717 | 63.926 | 1.00 36.72 |
| ATOM | 3940 | C | PHE B | | 47.929 | -7.508 | 61.456 | 1.00 26.43 |
| | | | | | | | | |
| MOTA | 3941 | 0 | PHE B | | 48.689 | -8.061 | 60.669 | 1.00 27.61 |
| ATOM | 3942 | N | LEU B | 118 | 46.642 | -7.809 | 61.551 | 1.00 23.59 |
| ATOM | 3943 | CA | LEU B | 118 | 46.048 | -8.820 | 60.705 | 1.00 29.15 |
| ATOM | 3944 | CB | LEU B | | 44.585 | | | |
| | | | | | | -9.039 | 61.099 | 1.00 28.78 |
| ATOM | 3945 | CG | LEU B | | 44.375 | -9.478 | 62.557 | 1.00 35.24 |
| ATOM | 3946 | CD1 | LEU B | 118 | 42.898 | -9.763 | 62.788 | 1.00 31.92 |
| ATOM | 3947 | CD2 | LEU B | 118 | 45.205 | -10.723 | 62.856 | 1.00 33.40 |
| ATOM | 3948 | c | LEU B | | 46.153 | | | |
| | | | | | | -8.422 | 59.236 | 1.00 30.15 |
| ATOM | 3949 | 0 | LEU B | | 46.350 | -9.276 | 58.379 | 1.00 27.04 |
| ATOM | 3950 | N | LYS B | 119 | 46.035 | -7.128 | 58.947 | 1.00 27.96 |
| ATOM | 3951 | CA | LYS B | 119 | 46.127 | -6.663 | 57.569 | 1.00 26.69 |
| ATOM | 3952 | СВ | | | | | | |
| | | | LYS B | | 45.470 | -5.291 | 57.412 | 1.00 23.94 |
| MOTA | 3953 | CG | LYS B | | 43.998 | -5.260 | 57.795 | 1.00 24.41 |
| ATOM | 3954 | CD | LYS B | 119 | 43.327 | -3.970 | 57.350 | 1.00 27.53 |
| ATOM | 3955 | CE | LYS B | 119 | 44.024 | -2.739 | 57.886 | 1.00 33.13 |
| | 3956 | | LYS B | | | | | |
| ATOM | | NZ | | | 43.371 | -1.479 | 57.428 | 1.00 27.75 |
| atom | 3957 | С | LYS B | 119 | 47.577 | -6.598 | 57.101 | 1.00 29.12 |
| ATOM | 3958 | 0 | LYS B | 119 | 47.864 | -6.160 | 55.984 | 1.00 35.25 |
| ATOM | 3959 | N | GLY B | | 48.493 | -7.034 | 57.958 | 1.00 30.25 |
| | | | | | | | | |
| MOTA | 3960 | CA | GLY B | | 49.896 | -7.037 | 57.585 | 1.00 28.38 |
| ATOM | 3961 | C | GLY B | 120 | 50.642 | -5.751 | 57.861 | 1.00 27.91 |
| MOTA | 3962 | 0 | GLY B | 120 | 51.775 | -5.582 | 57.403 | 1.00 22.25 |
| ATOM | 3963 | N | ASN B | | 50.024 | -4.836 | 58.600 | 1.00 25.42 |
| | | | | | | | | |
| MOTA | 3964 | CA | ASN B | | | 3.587 | 58.919 | 1.00 29.49 |
| MOTA | 3965 | CB | ASN B | 121 | 49.758 | -2.389 | 58.727 | 1.00 30.07 |
| ATOM | 3966 | CG | ASN B | 121 | 49.201 | -2.307 | 57.325 | 1.00 32.25 |
| ATOM | 3967 | OD1 | ASN B | | 49.924 | -2.491 | 56.350 | 1.00 35.44 |
| | | | | | | | | |
| MOTA | 3968 | ND2 | ASN B | 121 | 47.917 | -2.006 | | 1.00 32.26 |
| MOTA | 3969 | C | ASN B | 121 | 51.172 | -3.637 | 60.361 | 1.00 30.92 |
| ATOM | 3970 | 0 | ASN B | | 50.971 | -4.631 | 61.059 | 1.00 27.08 |
| | | | | | | | | |
| ATOM | 3971 | N | VAL B | | 51.810 | -2.560· | 60.796 | 1.00 28.46 |
| ATOM | 3972 | CA | VAL B | 122 | 52.309 | -2.457 | 62.155 | 1.00 29.48 |
| ATOM | 3973 | CB | VAL B | 122 | 53.840 | -2.35 2 | 62.177 | 1.00 33.40 |
| | 3974 | CG1 | VAL B | | 54.334 | -2.294 | 63.611 | 1.00 32.22 |
| MOTA | | | _ | | | -2.634 | | |
| ATOM | 3975 | CG2 | VAL B | | 54.446 | -3.544 | 61.458 | 1.00 33.57 |
| MOTA | 3976 | C | VAL B | 122 | 51.713 | -1.196 | 62.748 | 1.00 29.04 |
| ATOM | 3977 | O | VAL B | | 51.800 | -0.118 | 62.153 | 1.00 27.47 |
| | _ | | ALA B | | 51.100 | | 63.918 | 1.00 26.71 |
| ATOM | 3978 | N | | | | -1.326 | | |
| ATOM | 3979 | CA | YTY B | | 50.477 | ~0.177 | 64.559 | 1.00 25.62 |
| MOTA | 3980 | CB | ALA B | 123 | 48.963 | -0.281 | 64.447 | 1.00 21.65 |
| ATOM | 3981 | c | ALA B | | 50.872 | -0.005 | 66.017 | 1.00 28.62 |
| | | | _ | | | | | |
| ATOM | 3982 | 0 | ALA B | | 51.227 | -0.965 | 66.712 | 1.00 26.96 |
| MOTA | 3983 | N | PHE B | 124 | 50.805 | 1.239 | 66.472 | 1.00 22.85 |
| | | | | | | | | |

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Figure 18-61

| | | | | 2.4 | 51.122 | 1.577 | 67.847 | 1.00 17.31 |
|-------|-------|-----|----------|-------------|--------|--------|--------|------------|
| MOTA | 3984 | CA | PHE B 1 | | | 2.404 | 67.876 | 1.00 16.88 |
| ATOM | 3985 | CB | PHE B 1: | | 52.419 | | | 1.00 18.52 |
| ATOM | 3986 | CG | PHE B 1 | | 52.762 | 3.000 | 69.225 | |
| ATOM | 3987 | CD1 | PHE B 1 | 24 | 52.533 | 2.304 | 70.403 | 1.00 17.52 |
| ATOM | 3988 | CD2 | PHE B 1 | 24 | 53.382 | 4.245 | 69.297 | 1.00 17.88 |
| ATOM- | 3989 | CE1 | PHE B 1 | 24. | 52.914 | 2.837 | 71.638 | 1.00 25.77 |
| ATOM | 3990 | CE2 | PHE B 1 | | 53.769 | 4.790 | 70.517 | 1.00 21.97 |
| | 3991 | CZ | PHE B 1 | | 53.535 | 4.084 | 71.698 | 1.00 20.16 |
| MOTA | | | PHE B 1 | | 49.937 | 2.348 | 68.421 | 1.00 18.77 |
| MOTA | 3992 | C | PHE B 1 | | 49.462 | 3.311 | 67.820 | 1.00 16.62 |
| ATOM | 3993 | | | | 49.418 | 1.868 | 69.546 | 1.00 16.69 |
| MOTA | 3994 | N | ASN B 1 | | 48.320 | 2.528 | 70.238 | 1.00 16.22 |
| MOTA | 3995 | CA | ASN B 1 | | | 1.603 | 70.435 | 1.00 12.71 |
| ATOM | 3996 | CB | ASN B 1 | | 47.129 | _ | 71.346 | 1.00 19.79 |
| ATOM | 3997 | CG | ASN B 1 | | 46.095 | 2.209 | | 1.00 20.83 |
| ATOM | 3998 | OD1 | ASN B 1 | | 45.930 | 3.430 | 71.372 | 1.00 20.03 |
| MOTA | 3999 | ND2 | ASN B 1 | | 45.376 | 1.371 | 72.087 | |
| ATOM | 4000 | С | ASN B 1 | 25 | 48.790 | 3.004 | 71.600 | 1.00 19.19 |
| ATOM | 4001 | 0 | ASN B 1 | 25 · | 48.687 | 2.280 | 72.585 | 1.00 20.99 |
| ATOM | 4002 | N | PRO B 1 | 26 | 49.335 | 4.226 | 71.668 | 1.00 19.02 |
| ATOM | 4003 | CD | PRO B 1 | 26 | 49.595 | 5.156 | 70.555 | 1.00 21.39 |
| | 4004 | CA | PRO B 1 | | 49.833 | 4.805 | 72.917 | 1.00 21.60 |
| ATOM | 4005 | CB | PRO B 1 | | 50.398 | 6.161 | 72.459 | 1.00 21.07 |
| MOTA | | CG | PRO B 1 | | 49.530 | 6.487 | 71.269 | 1.00 17.70 |
| ATOM | 4006 | | PRO B 1 | | 48.808 | 4.942 | 74.034 | 1.00 20.69 |
| ATOM | 4007 | C | PRO B 1 | | 49.178 | 5.053 | 75.198 | 1.00 19.79 |
| MOTA | 4008 | 0 | | | 47.525 | 4.937 | 73.689 | 1.00 16.67 |
| ATOM | 4009 | N | ALA B 1 | | 46.476 | 5.065 | 74.698 | 1.00 20.44 |
| ATOM | 4010 | CA | ALA B 1 | | | 5.609 | 74.066 | 1.00 19.56 |
| ATOM | 4011 | CB | ALA B 1 | | 45.198 | | 75.401 | 1.00 20.80 |
| ATOM | 4012 | С | ALA B 1 | | 46.169 | 3.747 | 76.472 | 1.00 19.47 |
| ATOM | 4013 | 0 | ALA B 1 | | 45.555 | 3.742 | 74.800 | 1.00 20.52 |
| ATOM | 4014 | N | GLY B 1 | | 46.587 | 2.634 | - | 1.00 19.43 |
| ATOM | 4015 | CA | GLY B 1 | | 46.325 | 1.333 | 75.399 | |
| MOTA | 4016 | С | GLY B 1 | .28 | 47.327 | 0.910 | 76.463 | 1.00 20.56 |
| ATOM | 4017 | 0 | GLY B 1 | 28 . | 48.182 | 1.697 | 76.869 | 1.00 18.37 |
| ATOM | 4018 | N | GLY B 1 | .29 | 47.215 | -0.333 | 76.929 | 1.00 19.68 |
| ATOM | 4019 | CA | GLY B 1 | .29 | 48.136 | -0.820 | 77.943 | 1.00 19.93 |
| ATOM | 4020 | С | GLY B 1 | .29 | 47.620 | -0.619 | 79.358 | 1.00 25.25 |
| ATOM | 4021 | 0 | GLY B 1 | | 48.383 | -0.686 | 80.329 | 1.00 18.98 |
| ATOM | 4022 | N | MET B 1 | | 46.317 | -0.374 | 79.474 | 1.00 16.04 |
| ATOM | 4023 | CA | MET B 1 | | 45.677 | -0.161 | 80.768 | 1.00 19.26 |
| ATOM | 4024 | СВ | MET B 1 | | 44.301 | 0.451 | 80.519 | 1.00 17.94 |
| | 4025 | CG | MET B 1 | | 44.413 | 1.728 | 79.653 | 1.00 22.95 |
| MOTA | 4026 | SD | MET B 1 | | 42.873 | 2.615 | 79.307 | 1.00 31.83 |
| ATOM | 4027 | CE | MET B 1 | | 41.957 | 1.358 | 78.382 | 1.00 20.22 |
| ATOM | | | MET B 1 | | 45.598 | -1.548 | 81.421 | 1.00 22.63 |
| ATOM | 4028 | C | MET B 1 | | 44.546 | -2.173 | 81.486 | 1.00 16.24 |
| ATOM | 4029 | 0 | HIS B 1 | | 46.737 | -1.999 | 81.932 | 1.00 18.42 |
| ATOM | 4030 | N | | | 46.853 | -3.343 | 82.472 | 1.00 17.07 |
| ATOM | 4031 | CA | HIS B 1 | | 48.323 | | 82.341 | 1.00 17.61 |
| atom | 4032 | CB | HIS B 1 | | | -2.979 | 83.106 | 1.00 14.01 |
| ATOM | 4033 | CG | HIS B 1 | | 49.316 | -1.904 | 83.915 | 1.00 13.47 |
| atom | 4034 | | HIS B 1 | | 49.138 | | 83.051 | 1.00 18.00 |
| ATOM | 4035 | ND1 | HIS B 1 | 131 | 50.680 | -3.190 | 83.789 | 1.00 15.27 |
| ATOM | 4036 | CEl | HIS B 1 | 131 | 51.297 | -2.281 | | 1.00 17.21 |
| ATOM | 4037 | NE2 | HIS B 1 | 131 | 50.384 | -1.489 | 84.324 | |
| ATOM | 4038 | С | HIS B 1 | L 31 | 46.329 | -3.724 | 83.852 | 1.00 16.41 |
| ATOM | 4039 | 0 | HIS B 1 | 131 | 46.452 | -4.883 | 84.236 | 1.00 19.37 |
| ATOM | 4040 | N | HIS B 1 | 132 | 45.721 | -2.794 | 84.586 | 1.00 18.64 |
| | 4041 | CA | HIS B 1 | | 45.241 | -3.112 | 85.936 | 1.00 20.87 |
| ATOM | 4042 | CB | HIS B 1 | | 45.513 | -1.935 | 86.885 | 1.00 18.85 |
| ATOM | _ | CG | HIS B 1 | | 46.966 | -1.686 | 87.152 | 1.00 20.00 |
| ATOM | 1043 | CDJ | HIS B 1 | 132 | 47.715 | -0.563 | 87.030 | 1.00 15.74 |
| ATOM | 4044 | NO | HIS B 1 | 132 | 47.810 | -2.655 | 87.659 | 1.00 14.72 |
| ATOM | 4045 | MAT | HIS B 1 | 132 | 49.014 | -2.139 | 87.837 | 1.00 14.64 |
| atom | 4046 | CET | TIO D 1 | 132 | 48.984 | -0.872 | 87.462 | 1.00 14.88 |
| ATOM | 404.7 | | HIS B 1 | 122 | | -3.547 | 86.136 | 1.00 22.83 |
| ATOM | 4048 | C | HIS B 1 | 132 | 43.778 | -4.298 | 87.076 | 1.00 17.84 |
| ATOM | 4049 | 0 | HIS B 1 | 132 | 43.478 | -4.470 | 5 | |
| | | | | | | | | |

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| | 4050 | 87 | | | 42 02 | 0 2 000 | 05 271 | 1 00 15 54 |
|------|------|-----|--------|-------|--------|------------------|--------|-------------|
| ATOM | 4050 | N | ALA I | | 42.87 | | 85.271 | 1.00 16.54 |
| MOTA | 4051 | CA | ALA I | 3 133 | 41.45 | 7 -3.396 | 85.424 | 1.00 19.13 |
| ATOM | 4052 | CB | ALA I | 3 133 | 40.65 | 4 -2.704 | 84.328 | 1.00 23.56 |
| | | | | | | | 85.439 | 1.00 23.12 |
| ATOM | 4053 | C | ALA I | | 41.12 | | | |
| MOTA | 4054 | 0 | ALA I | 3 133 | 41.71 | B - 5.677 | 84.696 | 1.00 18.03 |
| ATOM | 4055 | N | PHE B | 3 134 | 40.18 | 1 -5.257 | 86.294 | 1.00 19.69 |
| | 4056 | CA | PHE E | | 39.76 | | 86.365 | 1.00 19.35 |
| ATOM | | | | | | | | |
| MOTA | 4057 | CB | PHE E | | 39.58 | | 87.818 | 1.00 21.26 |
| ATOM | 4058 | CG | PHE E | 3 134 | 40.83 | 7 -7.053 | 88.646 | 1.00 23.41 |
| ATOM | 4059 | CD1 | PHE E | 3 134 | 41.04 | 1 -6.009 | 89.544 | 1.00 24.25 |
| | 4060 | CD2 | | | 41.82 | | 88.522 | 1.00 22.80 |
| ATOM | | | | | | | | |
| ATOM | 4061 | CE1 | | | 42.20 | | 90.311 | 1.00 23.36 |
| ATOM | 4062 | CE2 | PHE F | 134 | 42.99 | 7 -7.964 | 89.283 | 1.00 27.74° |
| ATOM | 4063 | CZ | PHE E | 134 | 43.19 | -6.917 | 90.178 | 1.00 24.05 |
| | 4064 | C | PHE E | | 38.44 | | 85.621 | 1.00 18.60 |
| ATOM | | | | | | | | |
| MOTA | 4065 | 0 | PHE E | | 37.81 | | 85.196 | 1.00 13.82 |
| ATOM | 4066 | N | LYS E | 135 | 38.05 | -8.064 | 85.454 | 1.00 19.78 |
| ATOM | 4067 | CA | LYS E | 135 | 36.81 | 3 -8.421 | 84.782 | 1.00 28.09 |
| | 4068 | CB | LYS E | | 36.50 | | 85.125 | 1.00 34.06 |
| MOTA | | | | | | | | • |
| MOTA | 4069 | CG | LYS B | | | 7 -10.310 | 84.953 | 1.00 42.76 |
| MOTA | 4070 | CD | LYS B | 135 | 34.92 | 7 -11.745 | 85.437 | 1.00 48.44 |
| ATOM | 4071 | CE | LYS E | 135 | 33.46 | 2 -12.152 | 85.531 | 1.00 55.66 |
| | 4072 | NZ | LYS B | | | 7 -11.332 | 86.544 | 1.00 51.65 |
| MOTA | | | | | | | | |
| ATOM | 4073 | C | LYS B | | 35.639 | | 85.172 | 1.00 28.27 |
| MOTA | 4074 | 0 | LYS B | 135 | 34.92 | 7 -6.999 | 84.309 | 1.00 24.86 |
| MOTA | 4075 | N | SER B | 136 | 35.450 | 7.292 | 86.470 | 1.00 29.89 |
| | 4076 | CA | SER B | | 34.33 | | 86.933 | 1.00 30.86 |
| MOTA | | | | | | | | |
| MOTA | 4077 | CB | SER B | | 33.282 | | 87.582 | 1.00 31.57 |
| ATOM | 4078 | OG | SER B | 136 | 32.91 | -8.434 | 86.698 | 1.00 45.10 |
| ATOM | 4079 | C | SER B | 136 | 34.709 | -5.380 | 87.923 | 1.00 31.50 |
| | 4080 | 0 | SER B | 136 | 33.887 | -4.997 | 88.765 | 1.00 24.54 |
| ATOM | | | ARG B | | 35.920 | | 87.835 | 1.00 22.63 |
| MOTA | 4081 | N | | | | | | |
| ATOM | 4082 | CA | ARG B | | 36.291 | | 88.794 | 1.00 25.51 |
| ATOM | 4083 | CB | ARG B | 137 | 36.629 | -4:486 | 90.136 | 1.00 29.62 |
| ATOM | 4084 | CG | ARG B | 137 | 36.391 | -3.578 | 91.318 | 1.00 36.21 |
| | 4085 | CD | ARG B | | 36.874 | | 92.631 | 1.00 40.79 |
| ATOM | | | | | | | 93.744 | |
| MOTA | 4086 | NE | ARG B | | 36.36 | | | 1.00 45.95 |
| ATOM | 4087 | cz | ARG B | 137 | 36.863 | -3.369 | 94.973 | 1.00 41.97 |
| MOTA | 4088 | NH1 | ARG B | 137 | 37.897 | -4.144 | 95.263 | 1.00 43.42 |
| | 4089 | NH2 | ARG B | 137 | 36.322 | -2.604 | 95.913 | 1.00 46.65 |
| ATOM | | | ARG B | | 37.461 | | 88.339 | 1.00 24.73 |
| MOTA | 4090 | C | | | | | | |
| MOTA | 4091 | 0 | ARG B | | 38.420 | | 87.734 | 1.00 19.32 |
| MOTA | 4092 | N | ALA B | 138 | 37.372 | -1.663 | 88.631 | 1.00 16.77 |
| MOTA | 4093 | CA | ALA B | 138 | 38.428 | -0.733 | 88.270 | 1.00 18.50 |
| | 4094 | СВ | ALA B | | 37.939 | | 88.401 | 1.00 17.24 |
| ATOM | | | | | | | | 1.00 22.62 |
| ATOM | 4095 | С | ALA B | | 39.597 | | 89.216 | |
| MOTA | 4096 | 0 | ALA B | 138. | 39 411 | | 90.346 | 1.00 18.98 |
| MOTA | 4097 | N | ASN B | 139 | 40.301 | -0.641 | 88.759 | 1.00 20.82 |
| ATOM | 4098 | CA | ASN B | 139 | 41.989 | -0.828 | 89.585 | 1.00 25.17 |
| | | CB | ASN B | | 42.311 | | 89.689 | 1.00 20.59 |
| ATOM | 4099 | | | | | | | |
| MOTA | 4100 | CG | ASN B | 139 | 43.556 | -2.608 | 90.511 | 1.00 27.70 |
| ATOM | 4101 | OD1 | ASN B | 139 | 43.726 | -2.057 | 91.592 | 1.00 22.43 |
| ATOM | 4102 | ND2 | ASN B | 139 | 44.420 | -3.487 | 90.010 | 1.00 24.43 |
| | | C | ASN B | | 43.176 | | 89.020 | 1.00 22.37 |
| MOTA | 4103 | | | | | | | |
| ATOM | 4104 | | asn b | | 43.338 | | 87.799 | 1.00 17.50 |
| ATOM | 4105 | N | GLY B | 140 | 43.984 | 0.496 | 89.920 | 1.00 21.67 |
| ATOM | 4106 | CA | GLY B | | 45.166 | 1.249 | 89.524 | 1.00 23.06 |
| | | | GLY B | | 45.005 | 2.268 | 88.402 | 1.00 26.29 |
| ATOM | 4107 | | | | | | | 1.00 22.47 |
| ATOM | 4108 | | GLY B | | 45.827 | 2.301 | 87.479 | 1.00 22.47 |
| MOTA | 4109 | N | PHE B | 141 | 43.958 | 3.093 | 88.473 | 1.00 22.33 |
| | 4110 | CA | PHE B | 141 | 43.694 | 4.126 | 87.461 | 1.00 19.01 |
| ATOM | | CB | PHE B | 141 | 44.996 | 4.806 | 86.997 | 1.00 22.90 |
| MOTA | 4111 | CD | EITH D | 7.41 | | | 88.097 | 1.00 23.17 |
| ATOM | 4112 | CG | PHE B | 7 4 T | 45.810 | 5.433 | | 1.00 23.17 |
| ATOM | 4113 | CD1 | PHE B | 141 | 47.114 | 5.851 | 87.842 | 1.00 22.17 |
| | 4114 | CD2 | PHE B | 141 | 45.281 | 5.635 | 89.366 | 1.00 23.40 |
| ATOM | 4115 | CEI | PHE B | 141 | 47.876 | 6.462 | 88.833 | 1.00 24.02 |
| MOTA | 4777 | | - 1111 | | 2, | | | |

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| ATOM | 4116 | CE2 | PHE B | 141 | 46.033 | 6.244 | 90.361 | 1.00 23.03 |
|--------------|--------------|----------|-------|-------|------------------|------------------|------------------|--------------------------|
| ATOM | 4117 | CZ | PHE B | | 47.335 | 6.658 | 90.092 | 1.00 25.15 |
| MOTA | 4118 | C | PHE B | | 43.029 | 3.538 | 86.214 | 1.00 23.69 |
| MOTA | 4119 | Ō | PHE B | | 42.596 | 4.283 | 85.335 | 1.00 18.88 |
| MOTA | 4120 | N | CYS B | | 42.962 | 2.211 | 86.122 | 1.00 15.03 |
| ATOM | 4121 | CA | | 142 . | 42.380 | 1.578 | 84.938 | 1.00 19.55 |
| ATOM | 4122 | CB | | 142 | 43.193 | 0.336 | 84.552 | 1.00 20.38 |
| MOTA | 4123 | SG | CYS B | | 44.933 | 0.662 | 84.190 | 1.00 37.40 |
| MOTA | 4124 | c | CYS B | | 40.923 | 1.171 | 85.098 | 1.00 22.77 |
| ATOM | 4125 | ŏ | CYS B | | 40.561 | 0.514 | 86.082 | 1.00 23.04 |
| ATOM | 4126 | N | TYR B | | 40.094 | 1.557 | 84.130 | 1.00 15.24 |
| ATOM | 4127 | CA | TYR B | | 38.675 | 1.194 | 84.155 | 1.00 21.97 |
| MOTA | 4128 | CB | TYR B | | 37.795 | 2.372 | 83.723 | 1.00 18.06 |
| ATOM | 4129 | CG | TYR B | | 38.016 | 3.622 | 84.535 | 1.00 24.34 |
| ATOM | 4130 | | TYR B | | 39.038 | 4.516 | 84.214 | 1.00 23.20 |
| ATOM | 4131 | CE1 | TYR B | | 39.265 | 5.658 | 84.991 | 1.00 27.42 |
| ATOM | 4132 | CD2 | TYR B | | 37.226 | 3.892 | 85.652 | 1.00 19.15 |
| ATOM | 4133 | CE2 | TYR B | | 37.441 | 5.023 | 86.432 | 1.00 21.92 |
| ATOM | 4134 | CZ | TYR B | | 38.458 | 5.900 | 86.099 | 1.00 23.94 |
| ATOM | 4135 | ОН | TYR B | | 38.655 | 7.015 | 86.877 | 1.00 22.37 |
| ATOM | 4136 | С | TYR B | | 38.431 | 0.008 | 83.218 | 1.00 19.91 |
| ATOM | 4137 | 0 | TYR B | 143 | 37.665 | -0.902 | 83.535 | 1.00 22.50 |
| ATOM | 4138 | N | ILE B | 144 | 39.083 | 0.026 | 82.061 | 1.00 19.20 |
| ATOM | 4139 | CA | ILE B | 144 | 38.938 | -1.055 | 81.082 | 1.00 19.68 |
| ATOM | 4140 | CB | ILE B | 144 | 38.282 | -0.528 | 79.787 | 1.00 20.26 |
| ATOM | 4141 | CG2 | ILE B | 144 | 38:151 | -1.649 | 78.760 | 1.00 15.37 |
| ATOM | 4142 | CG1 | ILE B | 144 | 36.901 | 0.053 | 80.113 | 1.00 20.93 |
| ATOM | 4143 | CD1 | ILE B | 144 | 36.198 | 0.697 | 78.917 | 1.00 23.75 |
| ATOM | 4144 | С | ILE B | | 40.320 | -1.627 | 80.774 | 1.00 22.78 |
| MOTA | 4145 | 0 | ILE B | | 41.281 | -0.873 | 80.600 | 1.00 22.01 |
| ATOM | 4146 | N | ASN B | | 40.422 | -2.956 | 80.723 | 1.00 23.18 |
| MOTA | 4147 | CA | ASN B | | 41.698 | -3.623 | 80.451 | 1.00 20.63 |
| MOTA | 4148 | CB | ASN B | | 41.778 | -4.935 | 81.243 | 1.00 17.81 |
| MOTA | 4149 | CG | ASN B | | 43.188 | -5.531 | 81.268 | 1.00 25.17 |
| MOTA | 4150 | | ASN B | | 43.804 | -5.742 | 80.227 | 1.00 23.63 1.00 22.69 |
| MOTA | 4151 | | ASN B | | 43.693 | -5.819 | 82.472 | 1.00 22.09 |
| MOTA | 4152 | C | ASN B | | 41.780 | -3.918 | 78.955 78.508 | 1.00 21.10 |
| ATOM | 4153 | 0 | ASN B | | 41.389 | -5.002 -2.968 | 78.177 | 1.00 17.00 |
| MOTA | 4154 | N | ASN B | | 42.293 42.367 | -3.175 | 76.733 | 1.00 19.71 |
| MOTA | 4155 | CA | ASN B | | 42.773 | -1.880 | 76.015 | 1.00 17.65 |
| ATOM | 4156 | CB CG | ASN B | | 44.196 | -1.458 | 76.306 | 1.00 19.86 |
| MOTA | 4157 4158 | | ASN B | | 45.109 | -1.735 | 75.532 | 1.00 20.27 |
| ATOM | 4159 | | ASN B | | 44.395 | -0.798 | 77.435 | 1.00 11.85 |
| ATOM | 4160 | C | ASN B | | 43.277 | -4.342 | 76.331 | 1.00 19.07 |
| MOTA MOTA | 4161 | 0 | ASN B | | 43.030 | -4.996 | 75.328 | 1.00 18.61 |
| ATOM | 4162 | N | PRO B | | 44.358 | -4.598 | 77.082 | 1.00 17.78 |
| ATOM | 4163 | CD | PRO B | | 44.953 | -3.919 | 78.240 | 1.00 18.13 |
| ATOM | 4164 | CA | PRO B | | 45.197 | -5.735 | 76.678 | 1.00 19.98 |
| MOTA | 4165 | CB | PRO B | 147 | 46.338 | -5.694 | 77.698 | 1.00 24.29 |
| ATOM | 4166 | CG | PRO B | | 46.425 | -4.201 | 78.020 | 1.00 26.27 |
| MOTA | 4167 | C | PRO B | | 44.377 | -7.041 | 76.757 | 1.00 20.91 |
| ATOM | 4168 | 0 | PRO B | | 44.461 | -7.892 | 75.871 | 1.00 17.58 |
| ATOM | 4169 | N | ALA B | | 43.568 | -7.172 | .77.809 | 1.00 15.81 |
| ATOM | 4170 | CA | ALA B | 148 | 42.732 | -8.362 | 78.008 | 1.00 19.82 |
| ATOM | 4171 | CB | ALA B | | 42.049 | -8.312 | 79.372 | 1.00 17.50 |
| ATOM | 4172 | С | ALA B | | 41.683 | -8.473 | 76.903 | 1.00 22.58 |
| ATOM | 4173 | 0 | ALA B | 148 | 41.419 | -9.567 | 76.404 | 1.00 18.38 |
| ATOM | 4174 | N | VAL B | | 41.080 | -7.341 | 76.540 | 1.00 22.48 |
| ATOM | 4175 | CA | VAL B | | 40.086 | -7.300 | 75.466 | 1.00 19.04 |
| ATOM | 4176 | CB | VAL B | 149 | 39.503 | -5.877 | 75.281 | 1.00 18.96 |
| ATOM | 4177 | CG1 | VAL B | 149 | 38.691 | -5.800 | 73.988 | 1.00 17.32 |
| ATOM | 4178 | CG2 | VAL B | 149 | 38.621 | -5.531 | 76.462 | 1.00 15.33 |
| ATOM | 4179 | С | VAL B | | 40.763 | -7.709 | 74.166 | 1.00 22.12 |
| ATOM | 4180 | 0 | VAL B | | 40.240 | -8.535 | 73.421 73.903 | 1.00 21.83 |
| ATOM | 4181 | N | GLY B | 120 | 41.927 | -7.120 | 12.503 | 1.00 19.51 |

| | | | | | • | | | |
|---------------|------|-----|---------|-------|----------------|-----------------|--------|---------------------|
| ATOM | 4182 | CA | GLY B | 150 | 42.657 | -7.433 | 72.689 | 1.00 19.32 |
| MOTA | 4183 | С | | 150 | 43.033 | | 72.606 | 1.00 19.59 |
| | | | | | | | | |
| ATOM | 4184 | 0 | GLY B | 150 | 42.862 | | 71.568 | 1.00 22.28 |
| MOTA | 4185 | N | ILE B | 151 | 43.558 | -9.435 | 73.700 | 1.00 19.51 |
| ATOM | 4186 | CA: | ILE B | | 43 958 | -10.834 | 73.723 | 1.00 23.21 |
| | | | | | | | | |
| ATOM | 4187 | CB | ILE B | 151 | | -11.175 | 75.053 | 1.00 23.50 |
| ATOM | 4188 | CG2 | ILE B | 151 | 44.918 | -12.679 | 75.158 | 1.00 20.01 |
| ATOM | 4189 | CG1 | _ | 151 | 45.988 | | 75.129 | 1.00 21.98 |
| | | | | | | | | |
| ATOM | 4190 | CD1 | ILE B | 151 | | -10.502 | 76.457 | 1.00 21.24 |
| MOTA | 4191 | С | ILE B | 151 | 42.749 | -11.741 | 73.490 | 1.00 28.40 |
| ATOM | 4192 | 0 | ILE B | 151 . | 42.832 | -12.692 | 72.706 | 1.00 22.96 |
| | | | | | | -11.450 | 74.144 | 1.00 27.32 |
| ATOM | 4193 | N | | 152 | . — . | | | |
| MOTA | 4194 | CA | GLU B | 152 | 40.417 | -12.265 | 73.939 | 1.00 27.62 |
| ATOM | 4195 | CB | GLU B | 152 | 39.294 | -11.845 | 74.886 | 1.00 26.46 |
| ATOM | 4196 | -CG | GLU B | | 39.533 | -12.200 | 76.347 | 1.00 28.26 |
| | | | | | | | 76.592 | 1.00 31.10 |
| MOTA | 4197 | CD | | 152 | 39.613 | | | |
| ATOM | 4198 | OE1 | . GLU B | 152 | 39.668 | -14.123 | 77.767 | 1.00 29.55 |
| ATOM | 4199 | OE2 | GLU B | 152 | 39.626 | -14.481 | 75.617 | 1.00 30.51 |
| ATOM | 4200 | С | GLU B | | 39.948 | -12.125 | 72.497 | 1.00 30.30 |
| | | | | , | 39.463 | | | |
| MOTA | 4201 | 0 | | 152 | | | 71.893 | 1.00 25.58 |
| ATOM | 4202 | N | TYR B | 153 | 40.093 | -10.923 | 71.948 | 1.00 26.23 |
| ATOM | 4203 | CA | TYR B | 153 | 39.720 | -10.669 | 70.563 | 1.00 28.19 |
| ATOM | 4204 | CB | TYR B | | 40.082 | -9.235 | 70.190 | 1.00 27.94 |
| | | | | | 39.879 | | 68.735 | |
| ATOM | 4205 | CG | TYR B | | | -8.886 | | 1.00 28.46 |
| ATOM | 4206 | CD1 | TYR B | 153 | 38.618 | -8.560 | 68.240 | 1.00 25.69 |
| ATOM | 4207 | CE1 | TYR B | 153 | 38.447 | -8.195 | 66.898 | 1.00 30.73 |
| ATOM | 4208 | CD2 | | | 40.962 | -8.847 | 67,856 | 1.00 24.82 |
| | | | | | | -8.488 | 66.526 | 1.00 29.26 |
| ATOM | 4209 | CE2 | | | | | | |
| ATOM | 4210 | CZ | TYR B | 153 | 39.547 | -8.161 | 66.054 | 1.00 31.25 |
| ATOM | 4211 | OH | TYR B | 153 | 39.406 | -7.803 | 64.735 | 1.00 34.22 |
| ATOM | 4212 | С | TYR- B | 153 | 40.513 | -11.627 | 69.674 | 1.00 28.11 |
| | 4213 | ō | | 153 | | -12.248 | 68.759 | 1.00 22.06 |
| MOTA | | | | | | | | |
| ATOM | 4214 | N | LEU B | | | -11.725 | 69.944 | 1.00 26.77 |
| ATOM | 4215 | ,CA | LEU B | 154 | 42.681 | -12.:597 | 69.168 | 1.00 28.79 |
| MOTA | 4216 | CB | LEU B | 154 | 44.142 | -12.386 | 69.592 | 1.00 28.06 |
| ATOM | 4217 | CG | | 154 | 44.789 | -11.087 | 69.083 | 1.00 27.71 |
| - | | | | | | -10.860 | 69.759 | 1.00 34.15 |
| MOTA | 4218 | | | 154 | | | | |
| ATOM | 4219 | CD2 | | 154 | | -11.171 | 67.571 | 1.00 26.71 |
| ATOM | 4220 | C | LEU B | 154 | 42.299 | -14.074 | 69.274 | 1.00 26 <i>.</i> 98 |
| ATOM | 4221 | 0 | LEU B | 154 | 42.282 | -14.787 | 68.271 | 1.00 29.88 |
| | 1222 | N | ARG B | | | -14.536 | 70.480 | 1.00 23.19 |
| ATOM | | | | | | | | |
| ATOM | 4223 | CA | ARG B | | | -15.936 | 70.669 | 1.00 29.47 |
| ATOM | 4224 | CB | ARG B | 155 | 41.339 | -16.23 0 | 72.144 | 1.00 28.53 |
| ATOM | 4225 | CG | ARG B | 155 | 42.527 | -15.965 | 73.053 | 1.00 35.03 |
| ATOM | 4226 | CD | ARG B | | | -16.276 | 74.507 | 1.00 39.42 |
| | | | | | | -17.706 | 74.792 | 1.00 30.99 |
| ATOM | 4227 | NE | ARG B | | | | | |
| ATOM | 4228 | CZ | ARG B | | | -18.209 | 75.986 | 1.00 41.33 |
| MOTA | 4229 | NHI | | 155 | 41.591 | -17.394 | 77.002 | 1.00 38.47 |
| ATOM | 4230 | NH2 | ARG B | 155 | 41.872 | -19.523 | 76.178 | 1.00 40.67 |
| | 1231 | C | ARG B | | | -16.260 | 69.832 | 1.00 29.07 |
| ATOM | | | | | | | | |
| ATOM | 4232 | 0 | ARG B | | | -17.311 | | |
| ATOM | 4233 | N | LYS B | 156 | 39.41 9 | -15.357 | 69.828 | 1.00 28.99 |
| ATOM | 4234 | CA | LYS B | 156 | 38.216 | -15.573 | 69.038 | 1.00 34.63 |
| | | | LYS B | | | -14.534 | 69.386 | 1.00 36.63 |
| ATOM | 4235 | CB | | | | | | |
| ATOM | 4236 | CG | LYS B | | | -14.883 | 70.646 | 1.00 42.18 |
| λ TCM | 4237 | CD. | LYS B | | 37.292 | -14.900 | 71.868 | 1.00 51.38 |
| ATOM | 4238 | CE | LYS B | | 36.685 | -15.712 | 73.009 | 1.00 52.76 |
| | 4239 | | LYS B | | | -17.172 | 72.677 | 1.00 51.29 |
| ATOM | | NZ | | | | | | 1.00 34.66 |
| ATOM. | 4240 | С | LYS B | | | -15.562 | 67.538 | |
| TOM | 4241 | 0 | LYS B | 156 | | -16.088 | 66.754 | 1.60 33.53 |
| TCM | 4242 | N | LYS B | 157 | 39.625 | -14.966 | 67.140 | 1.00 30.06 |
| | -243 | CA | LYS B | | | -14.945 | 65.734 | 1.00 31.36 |
| ATOM | | | | | | -13.746 | 65.418 | 1.00 29.79 |
| ATCM | 1244 | CB | LYS B | | | | | 1 00 21 67 |
| ATOM | 4245 | CG | LYS B | | | -12.426 | 65.359 | 1.00 31.52 |
| ATOM | 4246 | CD | LYS B | 157 | 39.1 32 | -12.424 | 64.239 | 1.00 28.48 |
| | 4247 | CE | LYS B | | | -11.101 | 64.171 | 1.00 31.90 |
| ATOM | 2721 | | | | | ***- | | |

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MOTA 37.406 -11.980 4248 NZ LYS B 157 63.054 1.00 32.91 4249 65.381 LYS B 157 40.724 -16.234 1.00 31.92 C MOTA 4250 0 B 157 41.146 -16.421 64.246 1.00 ATOM LYS 33.58 4251 **GLY B 158** 40.890 -17.111 66.368 N 1.00 28.97 MOTA 4252 41.546 -18.379 66.112 ATOM CA **GLY B 158** 1.00 28.98 ATOM 4253 C **GLY B 158** 42.962 -18.569 66.622 1.00 33.33 43.503 -19.672 66.522 1.00 0 **GLY B 158** 30.58 4254 ATOM 4255 N PHE B 159 43.578 -17.521 67.164 1.00 32.80 ATOM 4256 CA PHE B. 159 44.937 -17.657 67.678 1.00 28.89 ATOM 45.560 -16.286 67.934 4257 CB -PHE B 159 1.00 30.33 ATOM PHE B 159 ATOM 4258 CG 45.748 -15.470 66.692 1.00 28:53 4259 44.682 -14.787 66.121 CD1 PHE B 159 1.00 24.58 ATOM 66.068 4260 CD2 PHE B 159 46.989 -15.420 1.00 24.21 ATOM ATOM 4261 CE1 PHE B 159 44.849 -14.066 64.948 1.00 25.26 64.895 1.00 23.66 CE2 PHE B 159 47.168 -14.706 4262 ATOM 4263 czPHE B 159 46.095 -14.026 64.332 1.00 26.65 ATOM 68.958 ATOM 4264 C PHE B 159 44.969 -18.484 1.00 30.92 69.820 4265 O PHE B 159 44.102 -18.334 1.00 24.26 MOTA ATOM 4266 N LYS B 160 45.979 -19.347 69.077 1.00 28.86 4267 CA LYS B 160 46.123 -20.224 70.237 1.00 30.27 ATOM 46.085 -21.692 4268 LYS B 160 69.800 1.00 32.05 CB MOTA 44.806 -22.117 ATOM 4269 CG LYS B 160 69.113 1.00 41.13 4270 CD LYS B 160 44.809 -23.621 68.826 1.00 40.73 ATOM 45.945 -24.031 4271 LYS B 160 67.904 1.00 43.16 CE ATOM 66:554 ATOM 4272 NZ LYS B 160 45.812 -23.408 1.00 48.69 4273 LYS B 160 47.394 -19.997 71.048 1.00 28.23 ATOM 4274 O LYS B 160 47.552 -20.561 72.130 1.00 25.29 ATOM 70.520 B 161 48.320 -19.206 1.00 28.51 ATOM 4275 N ARG 4276 CA ARG B 161 49.550 -18.921 71.247 1.00 25.84 ATOM 70.667 4277 CB ARG B 161 50.724 -19.719 1.00 25.33 MOTA 50.551 -21.245 70.781 1.00 27.47 4278 ARG B 161 ATOM CG 1.00 4279 CD ARG B 161 51.833 -21.985 70.394 32.27 MOTA ARG B 161 52.218 -21.761 69.002 1.00 34.90 ATOM 4280 NE 4281 ARG B 161 51.584 -22:276 67.954 1.00 38.45 CZ MOTA 50.527 -23.056 68.130 1.00 38.77 ATOM 4282 NH1 ARG B 161 66.725 4283 NH2 ARG B 161 51.999 -22.000 1.00 38.64 ATOM 49.818 -17.421 71.182 1.00 30.40 4284 ARG B 161 С ATOM ARG B 161 4285 50.393 -16.912 70.218 1.00 27.50 ATOM n 49.376 -16.722 72.221 1.00 4286 N ILE B 162 25.64 ATOM ILE B 162 49.515 -15.273 72.303 1.00 27.44 4287 CA MOTA 4288 72.545 CB ILE B 162 48.134 - 14.618 1.00 24.53 ATOM ILE B 162 48.249 -13.101 72.473 1.00 25.49 ATOM 4289 CG2 4290 CG1 ILE B 162 47.142 -15.101 71.487 1.00 29.46 ATOM 45.688 -14.707 71.758 1.00 4291 CD1 ILE B 162 31.94 ATOM 50.465 -14.868 1.00 22.68 \sim ILE B 162 73.429 ATOM 4292 74.568 1.00 24.25 4293 0 ILE B 162 5^.311 -15.302 ATOM LEU B 163 5..454 -14.042 73.100 1.00 19.49 ATOM 4294 N 51.425 -13.561 1.00 17.57 4295 CA **LEU B 163** 74.081 ATOM 73.528 1.00 20.54 4296 CB LEU B 163 53.850 -13.686 ATOM 4297 CG **LEU B 163** 54.979 -12.975 74.295 1.00 18.84 ATOM LEU B 163 55.102 -13.538 CD1 75.690 1.00 20.55 ATOM 4298 73.556 1.00 18.57 4299 CD2 LEU B 163 56.293 -13.148 ATOM LEU B 163 52.158 -12.099 74.430 1.00 16.20 4300 С ATOM 51.898 -11.277 LEU B 163 73.549 1.00 16.09 O ATOM 4301 75.715 4302 TYR B 164 52.227 -11.780 1.00 14.05 Ν ATOM TYR B 164 52.027 -10.411 76.191 1.00 16.21 4303 CA ATOM TYR B 164 50.777 -10.323 77.070 1.00 16.01 СЭ 4304 ATOM 1.00 15.08 4305 77.667 CG TYR B 164 50.534 -8.948 MOTA TYR B 164 4306 50.148 -7.869 76.869 1.00 19.51 CD1 ATOM TYR 5 164 49.948 77.418 1.00 12.88 -6.5974307 CE1 ATOM 79.021 1.00 14.07 50.715 4308 CD2 TYR B 164 -8.724ATOM TYR B 79.583 1.00 13.66 4309 CE2 164 50.520 -7.463 ATOM TYR B 164 78.782 1.00 14.72 4310 CZ50.139 -6.407- TOM 1.00 13.54 TYR B .164 49.952 -5.163 79.354 4311 OH ATOM 4312 C TYR B 164 53.246 -10.017 77.018 1.00 19.14 ROTE TYR B 164 53.539 -10.642 78.03*6* 1.00 26.51 4313 0 ATOM

| MOTA | 4314 | N | ILE B | 165 | 53.964 | -8.992 | 76.573 | 1.00 22.40 |
|------|------|------|-------|-------|---------|--------|--------|------------|
| | | | ILE B | | 55.148 | -8.518 | 77.285 | 1.00 17.72 |
| MOTA | 4315 | CA | | | | | | 1.00 22.51 |
| MOTA | 4316 | CB - | ILE B | 165 | 56.352 | -8.465 | 76.343 | |
| ATOM | 4317 | CG2 | ILE B | 165 | 57.582 | -7.902 | 77.079 | 1,00 16.36 |
| | | | ILE B | | 56.632 | -9.880 | 75.818 | 1.00 19.82 |
| MOTA | 4318 | CG1 | | | | | | |
| ATOM | 4319 | CD1 | ILE B | 165 | 57.721 | -9.942 | 74.742 | 1.00 21.74 |
| ATOM | 4320 | C | ILE B | 165 | 54.851 | -7.126 | 77.850 | 1.00 22.54 |
| | | | ILE B | | 54.478 | -6.223 | 77.111 | 1.00 16.60 |
| MOTA | 4321 | Ο, | | | | | | 1.00 15.78 |
| ATOM | 4322 | N | ASP B | 166 | 55.046 | -6.961 | 79.156 | |
| - | 4323 | CA | ASP B | 166 | 54.740 | -5.704 | 79.840 | 1.00 20.62 |
| MOTA | | | | | 53.719 | -5.996 | 80.949 | 1.00 17.57 |
| ATOM | 4324 | CB | ASP B | | | | | 1.00 25.39 |
| MOTA | 4325 | CG | ASP B | | 53,.063 | -4.742 | 81.486 | |
| | 4326 | 001 | ASP B | 166 | 53.779 | -3.859 | 82.003 | 1.00 19.68 |
| ATOM | | | ASP B | | 51.824 | -4.637 | 81.377 | 1.00 29.22 |
| ATOM | 4327 | OD2 | | | | | | 1.00 19.01 |
| ATOM | 4328 | C | ASP B | 166 | 55.976 | | 80.423 | |
| ATOM | 4329 | 0 | ASP B | 166 | 56.509 | -5.412 | 81.456 | 1.00 19.74 |
| | | | LEU B | | 56.414 | -3.923 | 79.775 | 1.00 17.88 |
| ATOM | 4330 | N | | | | -3.211 | 80.235 | 1.00 14.99 |
| ATOM | 4331 | CA | LEU B | | 57.598 | -3.211 | | |
| ATOM | 4332 | CB | LEU B | 167 | 58.412 | -2.710 | 79.044 | 1.00 19.22 |
| | | CG | LEU B | | 58.871 | -3.799 | 78.069 | 1.00 22.68 |
| MOTA | 4333 | | | | | | 77.074 | 1.00 25.35 |
| ATOM | 4334 | | LEU B | | 59.835 | -3.179 | | |
| ATOM | 4335 | CD2 | LEU B | 167 | 59.570 | -4.943 | 78.808 | 1.00 17.54 |
| | 4336 | С | LEU B | | 57.284 | -2.059 | 81.183 | 1.00 17.49 |
| ATOM | | | | | | -1.359 | 81.639 | 1.00 13.39 |
| MOTA | 4337 | 0 | LEU B | | 58.189 | | | |
| ATOM | 4338 | N | ASP B | 168 | 56.003 | -1.878 | 81.479 | 1.00 20.03 |
| | 4339 | CA | ASP B | 168 | 55.549 | -0.848 | 82.412 | 1.00 21.98 |
| MOTA | | | | | 54.030 | -0.955 | 82.597 | 1.00 21.21 |
| MOTA | 4340 | CB | ASP B | | | | | 1.00 24.92 |
| ATOM | 4341 | CG | ASP B | 168 | 53.453 | 0.186 | 83.428 | |
| ATOM | 4342 | С | ASP B | 168 | 56.241 | -1.139 | 83.753 | 1.00 22.98 |
| | - | | ASP B | | 56.447 | -2.304 | 84.091 | 1.00 18.36 |
| MOTA | 4343 | 0 | | | | | 82.825 | 1.00 22.03 |
| ATOM | 4344 | ODI | ASP B | 168 | 52.849 | 1.099 | | |
| ATOM | 4345 | OD2 | ASP B | 168 | 53.606 | 0.189 | 84.676 | 1.00 18.43 |
| | 4346 | N | ALA B | | 56.581 | -0.095 | 84.514 | 1.00 15.46 |
| ATOM | | | | | | -0.268 | 85.807 | 1.00 18.73 |
| ATOM | 4347 | CA | ALA B | 169 - | 57.263 | | | |
| ATOM | 4348 | CB | ALA B | 169 | 57.764 | 1.084 | 86.323 | 1.00 11.98 |
| ATOM | 4349 | С | ALA B | 169 | 56.400 | -0.940 | 86.886 | 1.00 21.82 |
| | | | ALA B | | 56.886 | -1.262 | 87.980 | 1.00 22.51 |
| MOTA | 4350 | 0 | | | | | 86.600 | 1.00 18.75 |
| ATOM | 4351 | N | HIS B | | 55.120 | -1.134 | | |
| ATOM | 4352 | CA | HIS B | 170 | 54.238 | -1.776 | 87.570 | 1.00 22.70 |
| | | c | HIS B | | 53.716 | -3.096 | 87.015 | 1.00 22.11 |
| ATOM | 4353 | | | | | -3.244 | 85.809 | 1.00 21.94 |
| ATOM | 4354 | 0 | HIS B | | 53.536 | | | |
| MOTA | 4355 | CB | HIS B | 170 | 53.050 | -0.867 | 87.927 | 1.00 21.28 |
| - | 4356 | CG | HIS B | 170 | 53.449 | 0.475 | 88.460 | 1.00 18.89 |
| MOTA | | | | | 53.695 | 1.539 | 87.626 | 1.00 19.13 |
| ATOM | 4357 | | HIS B | | | | 88.412 | 1.00 19.41 |
| MOTA | 4358 | CE1 | HIS B | 170 | 54.046 | 2.539 | | |
| ATOM | 4359 | CD2 | HIS B | 170 | 53.660 | 0.854 | 89.746 | 1.00 19.02 |
| | | | HIS B | | 54.042 | 2.174 | 89.710 | 1.00 20.45 |
| ATOM | 4360 | | | | | -4.047 | 87.907 | 1.00 19.20 |
| ATOM | 4361 | N | HIS B | | 53.474 | | | |
| ATOM | 4362 | CA | HIS B | 171 | 52.961 | -5.352 | 87.519 | 1.00 21.20 |
| | 4363 | CB | HIS B | 171 | 52.964 | -6.284 | 88.722 | 1.00 22.00 |
| ATOM | | | | | | -7.683 | 88.400 | 1.00 24.64 |
| ATOM | 4364 | CG | HIS B | | 52.541 | -,.003 | | |
| ATOM | 4365 | CD2 | HIS B | 171 | 53.056 | -8.594 | 87.540 | 1.00 19.19 |
| | 4366 | ירוא | HIS B | 171 | 51.441 | -8.279 | 88.979 | 1.00 25.71 |
| MOTA | | CD3 | urc p | 171 | 51.295 | -9.497 | 88.487 | 1.00 25.30 |
| MOTA | 4367 | CET | HIS B | 1/1 | | | 87.612 | 1.00 24.71 |
| ATOM | 4368 | NE2 | HIS B | 171 | 52.261 | -9.713 | | |
| MOTA | 4369 | С | HIS B | 171 | 51.549 | -5.306 | 86.943 | 1.00 23.91 |
| | | | HIS B | | 50.677 | -4.620 | 87.479 | 1:00 18.93 |
| atom | 4370 | 0 | | | | | 85.865 | 1.00 15.36 |
| MOTA | 4371 | N | CYS.B | 1/2 | 51.332 | -6.062 | | |
| MOTA | 4372 | CA | CYS 3 | 172 | 50.036 | -6.141 | 85.207 | 1.00 20.03 |
| | | | CYS B | 172 | 50.240 | -6.534 | 83.732 | 1.00 22.46 |
| ATOM | 4373 | CB | C13 5 | 172 | | | 83.419 | 1.00 23.49 |
| ATOM | 4374 | SG | CYS B | 1/2 | 51.259 | -8.030 | | 1 00 10 05 |
| MOTA | 4375 | С | CYS B | 172 | 49.110 | -7.146 | 85.913 | 1.00 18.05 |
| | | ō | CYS B | 172 | 48.712 | -8.151 | 85.327 | 1.00 18.23 |
| atom | 4376 | | 200 0 | 173 | 48.767 | -6.871 | 87.170 | 1.00 16.78 |
| ATOM | 4377 | N | ASP B | 1/3 | | | | 1.00 18.81 |
| ATOM | 4378 | CA | ASP B | 173 | 47.909 | -7.776 | 87.928 | 1.00 10.01 |
| | 1379 | CB | ASP B | 173· | 47.638 | -7.236 | 89.344 | 1.00 20.39 |
| atom | 95.7 | | | | | | • | |

183/263 Figure 18-67

| MOTA | 4380 | CG | ASP | B 173 | 46.961 | -5.871 | 89.354 | 1.00 23.40 |
|------|-------|-----|---------|-------|--------|---------|--------|------------|
| ATOM | 4381 | | 1 ASP | | 46.564 | | 90.455 | 1.00 18.64 |
| | 4382 | | | | 46.834 | | 88.291 | 1.00 19.24 |
| MOTA | | | | B 173 | 46.595 | | 87.219 | 1.00 17.46 |
| MOTA | 4383 | | | | | | | |
| ATOM | 4384 | | | B 173 | 46.162 | | 87.224 | 1.00 15.53 |
| MOTA | 4385 | | | В 174 | 45.978 | | 86.580 | 1.00 13.46 |
| ATOM | 4386 | CA | | B 174 | 44.733 | -7.391 | 85.876 | 1.00 18.18 |
| ATOM | 4387 | С | GLY : | B 174 | 44.904 | -8.392 | 84.741 | 1.00 17.85 |
| MOTA | 4388 | 0 | GLY : | B 174 | 44.104 | -9.316 | 84.583 | 1.00 18.27 |
| ATOM | 4389 | | VAL | B 175 | 45.951 | | 83.943 | 1.00 16.14 |
| ATOM | 4390 | | | 3 175 | 46.206 | | 82.829 | 1.00 17.00 |
| ATOM | 4391 | CB | | 3 175 | 47.305 | | 81.902 | 1.00 27.22 |
| | 4392 | CG: | | | 47.533 | | 80,731 | 1.00 19.75 |
| MOTA | | | | | | | | |
| ATOM | 4393 | | 2 VAL 1 | | 46.896 | | 81.396 | 1.00 18.66 |
| MOTA | 4394 | C | | 3 175 | | -10.486 | 83.324 | 1.00 22.82 |
| ATOM | 4395 | O | | 3 175 | | -11.503 | 82.754 | 1.00 18.06 |
| ATOM | 4396 | N | | 176 | | -10.520 | 84.378 | 1.00 21.67 |
| ATOM | 4397 | CA | GLN I | 3 176 | 47.889 | -11.798 | 84.911 | 1.00 21.55 |
| ATOM | 4398 | CB | GLN H | 176 | 48.824 | -11.602 | 86.105 | 1.00 19.68 |
| ATOM | 4399 | CG | GLN I | 176 | 49.088 | -12.905 | 86.862 | 1.00 20.17 |
| ATOM | 4400 | CD | GLN F | 3 176 | 50.066 | -12.759 | 87.996 | 1.00 25.42 |
| ATOM | 4401 | OE | | | | -12.442 | 87.786 | 1.00 21.56 |
| ATOM | 4402 | NE2 | | | | -13.000 | 89.217 | 1.00 20.18 |
| | 4403 | C | GLN E | | | -12.630 | 85.348 | 1.00 24.78 |
| MOTA | 4404 | õ | GLN E | | | -13.817 | 85.057 | 1.00 22.91 |
| ATOM | | | GLU E | | | | 86.051 | 1.00 22.91 |
| ATOM | 4405 | N | | | | -12.007 | | |
| ATOM | 4406 | CA | GLU E | | | -12.727 | 86.523 | 1.00 27.01 |
| MOTA | 4407 | CB | GLU E | | | -11.825 | 87.394 | 1.00 24.73 |
| MOTA | 4408 | CG | GLU E | | | -12.581 | 88.138 | 1.00 37.46 |
| ATOM | 4409 | CD | GLU E | | | -11.676 | 88.987 | 1.00 42.48 |
| ATOM | 4410 | OE1 | | | | -11.002 | 88.432 | 1.00 44.35 |
| MOTA | 4411 | OE2 | GLU E | 177 | 41.993 | -11.627 | 90.213 | 1.00 45.63 |
| ATOM | 4412 | С | GLU B | 177 | 43.732 | -13.247 | 85.370 | 1.00 26.56 |
| ATOM | 4413 | 0 | GLU B | 177 | 43.240 | -14.375 | 85.408 | 1.00 27.71 |
| ATOM | 4414 | N | ALA E | 178 | 43.573 | -12.418 | 84.344 | 1.00 24.58 |
| ATOM | 4415 | CA | ALA B | | | -12.775 | 83.174 | 1.00 25.86 |
| ATOM | 4416 | CB | ALA B | | | -11.628 | 82.171 | 1.00 24.20 |
| ATOM | 4417 | c | ALA B | | | -14.054 | 82.485 | 1.00 25.72 |
| MOTA | 4418 | ō | ALA B | | | -14.838 | 82.036 | 1.00 22.38 |
| | 4419 | N | PHE B | | | -14.282 | 82.395 | 1.00 27.19 |
| MOTA | 4420 | CA | PHE B | | | -15.489 | 81.703 | 1.00 27.05 |
| MOTA | | | PHE B | | 45.714 | | 80.418 | 1.00 27.03 |
| ATOM | 4421 | CB | | | | | | |
| MOTA | 4422 | CG | PHE B | | | -14.020 | 79.644 | 1.00 20.36 |
| MOTA | 4423 | | PHE B | | | -12.687 | 79.735 | 1.00 25.23 |
| ATOM | 4424 | | PHE B | | | -14.332 | 78.902 | 1.00 19.22 |
| ATOM | 4425 | | PHE B | | | -11.6?7 | 79.102 | 1.00 19.25 |
| ATOM | 4426 | CE2 | PHE B | 179 | | -13.315 | 78.272 | 1.00 20.65 |
| ATOM | 4427 | CZ | PHE B | 179 | 43.528 | -12.0C1 | 78.374 | 1.00 25.64 |
| MOTA | 4428 | С | PHE B | 179 | 45.866 | -16.398 | 82.556 | 1.00 23.50 |
| ATOM | 4429 | 0 | PHE B | 179 | 46.652 | -17.182 | 82.038 | 1.00 18.26 |
| ATOM | 4430 | N | TYR B | 180 | | -16.313 | 83.868 | 1.00 23.24 |
| | 4431 | CA | TYR B | | | -17.106 | 84.799 | 1.00 26.76 |
| MOTA | 4432 | CB | TYR B | | | -16.665 | 86.231 | 1.00 25.72 |
| ATOM | 4433 | CG | TYR B | | | -16.969 | 87.247 | 1.00 29.66 |
| MOTA | | | TYR B | | | -17.942 | 88.237 | 1.00 27.07 |
| ATOM | 4434 | | | | - | | 89.170 | |
| ATOM | 4435 | CE1 | TYR B | | | -18.222 | | 1.00 30.08 |
| ATOM | 443,6 | CD2 | TYR B | | | -16.283 | 87.216 | 1.00 29.68 |
| ATCM | 4437 | CE2 | TYR B | | | -16.552 | 88.139 | 1.00 30.99 |
| ATOM | 4438 | CZ | TYR B | | | -17.521 | 89.112 | 1.00 33.16 |
| MOTA | 4439 | OH | TYR B | | 50.262 | -17.791 | 90.006 | 1.00 28.47 |
| ATOM | 4440 | С | TYR B | 180 | 46.256 | -18.619 | 84.649 | 1.00 29.13 |
| ATOM | 4441 | 0 | TYR B | 180 | | -19.416 | 84.922 | 1.00 23.43 |
| ATOM | 4442 | N | ASP B | 181 | | -19.021 | 84.190 | 1.00 25.67 |
| | 4443 | CA | ASP B | | | -20.445 | 84.075 | 1.00 28.28 |
| ATOM | 1444 | CB | ASP B | | | -20.759 | 84.757 | 1.00 32.13 |
| ATOM | | CG | ASP B | | | -20.410 | 83.890 | 1.00 36.12 |
| ATCM | 4445 | Ų. | | ~~~ | 47.741 | -20.410 | 000 | |

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| MOTA | 4446 | 5 OD1 ASP B 181 | 42.202 -19.300 | 83.329 | 1.00 41.04 |
|--------------|--------------|-----------------------------|----------------------------------|------------------|--------------------------|
| ATOM | 4447 | 7 OD2 ASP B 181 | 41.334 ~21.249 | | |
| MOTA | 4448 | 3 C ASP B 181 | | | 1.00 32.41 |
| MOTA | 4449 | O ASP B 181 | | | 1.00 31.67 |
| ATOM | 4450 | | | | 1.00 29.24 |
| ATOM | 4451 | | | | 1.00 30.57 |
| MOTA | 4452 | | 44.468 -20.008 | | 1.00 30.03 |
| ATOM | 4453 | | | | 1.00 28.22 |
| ATOM | 4454 | | 44.947 -18.561 | | 1.00 26.55 |
| ATOM | 4455 | | 46.759 -20.870 | | 1.00 20.33 |
| ATOM | 4456 | | - 47.591 -20.007 | - | 1.00 27.27 |
| ATOM | 4457 | | 46.999 -21.878 | 78.909 | 1.00 29.94 |
| ATOM | 4458 | | 48.296 -22.049 | 78.273 | 1.00 31.40 |
| ATOM | 4459 | | 48.648 -23.536 | 78.228 | 1.00 33.36 |
| ATOM | 4460 | • | 47.718 -24.319 | 77.328 | 1.00 33.33 |
| ATOM | 4461 | OD1 ASP B 183 | 46.513 -23.988 | 77.287 | 1.00 28.06 |
| ATOM | 4462 | OD2 ASP B 183 | 48.186 -25.271 | 76.675 | 1.00 38.19 |
| ATOM | 4463 | C ASP B 183 | 48.321 -21.462 | 76.864 | 1.00 31.14 |
| ATOM | 4464 | O ASP B 183 | 49.332 -21.557 | 76.168 | 1.00 28.74 |
| MOTA | 4465 | N GLN B 184 | 47.217 -20.852 | 76.446 | 1.00 25.34 |
| ATOM | 4466 | CA GLN B 184 | 47.151 -20.251 | 75.118 | 1.00 28.59 |
| ATOM | 4467 | CB GLN B 184 | 45.712 -20.256 | 74.581 | 1.00 26.84 |
| ATOM | 4468 | CG GLN B 184 | 45.060 -21.632 | 74.529 | 1.00 34.86 |
| ATOM | 4469 | CD GLN B 184 | 43.760 -21.647 | 73.736 | 1.00 32.27 |
| ATOM | 4470 | OE1 GLN B 184 | 42.897 -20.789 | 73.912 | 1.00 35.43 |
| MOTA | 4471 | NE2 GLN B 184 | 43.611 -22.641 | 72.870 | 1.00 28.92 |
| ATOM | 4472 | C GLN B 184 | 47.672 -18.817 | 75.175 | 1.00 27.28 |
| MOTA | 4473 | O GLN B 184 | 47.871 -18.171 | 74.148 | 1.00 29.70 |
| ATOM | 4474 | N VAL B 185 | 47.900 -18.325 | 76.386 | 1.00 27.64 |
| ATOM | 4475 | CA VAL B 185 | 48.400 -16.972 | 76.575 | 1.00 26.26 |
| ATOM | 4476 | CB VAL·B 185 | 47.304 -16.039 | 77.145 | 1.00 22.85 |
| ATOM | 4477 | CG1 VAL B 185 | 47.879 -14.642 | 77.395 | 1.00 23.10 |
| ATOM | 4478 | CG2 VAL B 185 | 46.136 -15.967 | 76.191 | 1.00 21.67 |
| ATOM | 4479 | C VAL B 185 | 49.570 -16.964 | 77.547 | 1.00 27.01 |
| ATOM | 4480 | O VAL B 185 | 49.456 -17.469 | 78.663 | 1.00 23.75 |
| ATOM | 4481 | N PHE B 186 CA PHE B 186 | 50.696 -16.403 | 77.115 | 1.00 22.02 |
| ATOM | 4482 4483 | | 51.868 -16.301 | 77.978 | 1.00 21.83 |
| ATOM ATOM | 4484 | CB PHE B 186 CG PHE B 186 | 53.142 -16.763 54.336 -16.921 | 77.252 78.170 | 1.00 17.02 |
| ATOM | 4485 | CD1 PHE B 186 | 54.756 -18.189 | 78.580 | 1.00 24.84 1.00 22.70 |
| ATOM | 4486 | CD2 PHE B 186 | 55.004 -15.805 | 78.670 | 1.00 20.26 |
| ATOM | 4487 | CE1 PHE B 186 | 55.819 -18.338 | 79.471 | 1.00 20.20 |
| ATOM | 4488 | CE2 PHE B 186 | 56.071 -15.941 | 79.563 | 1.00 20.01 |
| ATOM | 4489 | CZ PHE B 186 | 56.481 -17.206 | 79.968 | 1.00 17.84 |
| ATOM | 4490 | C PHE B 186 | 52.032 -14.827 | 78.368 | 1.00 18.12 |
| ATO: | 4491 | O PHE B 186 | 52.038 -13.946 | 77.508 | 1.00 15.92 |
| MOTA | 4492 | N VAL B 187 | 52.161 -14.565 | 79.661 | 1.00 18.06 |
| ATOm | 4493 | CA VAL B 187 | 52.348 -13.208 | 80.153 | 1.00 17.67 |
| ATOM | 4494 | CB VAL B 187 | 51.282 -12.839 | 81.225 | 1.00 22.85 |
| MOTA | 4495 | CG1 VAL B 187 | 51.608 -11.473 | 81.840 | 1.00 24.08 |
| ATOM | 4496 | CG2 VAL B 187 | 49.882 -12.808 | 80.598 | 1.00 18.82 |
| ATOM | 4497 | C VAL B 187 | 53.735 -13.060 | 80.788 | 1.00 18.32 |
| ATOM | 4498 | O VAL B 187 | 54.092 -13.807 | 81.707 | 1.00 18.82 |
| ATOM | 4499 | N LEU B 188 | 54.503 -12.103 | 80.282 | 1.00 14.70 |
| MOTA | 4500 | CA LEU B 188 | 55.832 -11.789 | 80.798 | 1.00 18.84 |
| ATCM | 4501 | CB LEU B 188 | 56.900 -11.948 | 79.716 | 1.00 18.64 |
| MOTA | 4502 | CG LEU B 188 | 58.230 -11.277 | 80.082 | 1.00 21.23 |
| ATOM | 4503 | CD1 LEU B 188 | 58.769 -11.832 | 81.395 | 1.00 18.55 |
| MOTA | 4504 | CD2 LEU B 188 | 59.227 -11.489 | 78.957 | 1.00 20.49 |
| ATOM | 4505 | C LEU B 188 | 55.836 -10.339 | 81.280 | 1.00 22.14 |
| ATOM | 4506 | O LEU B 188 | 55.527 -9.410 | 80.517 | 1.00 19.96 |
| ATOM | 4507 | N SER B 189 | 56.187 -10.133 | | 1.00 21.08 |
| ATOM | 4508 | CA SER B 189 | 56.203 -8.782 | | 1.00 21.85 |
| ATOM | 4509 | CB SER B 189 | 54.956 -8.543 | | 1.00 25.95 |
| ATCM | 4510 | OG SER B 189 | 54.988 -7.252 | | 1.00 21.91 |
| ATOM | 4511 | C SER B 189 | 57.423 -8.420 | 83.883 | 1.00 23.62 |

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| ATOM | 4512 | 0 | .SER B 1 | 0.0 | 57.829 | -9.174 | 84.766 | 1 00 10 61 |
|--------|-------|-----|-----------------|------|--------|--------|--------|------------|
| | | | | | | | | 1.00 18.61 |
| ATOM | 4513 | | LEU B 1 | | 58.020 | -7.269 | 83.569 | 1.00 20.83 |
| ATOM | 4514 | CA | LEU B 1 | .90 | 59.149 | -6.767 | 84.347 | 1.00 21.85 |
| ATOM | 4515 | CB | LEU B 1 | 90 | 60.278 | ~6.226 | 83.473 | 1.00 22.85 |
| | 4516 | | | 90 | | -7.089 | 82.413 | • |
| ATOM | | | | | 60.964 | | | 1.00 32.59 |
| MOTA | 4517 | | | 90 | 62.337 | -6.479 | 82.140 | 1.00 29.27 |
| MOTA | 4518 | CD | LEU B 1 | 90 | 61.136 | -8.511 | 82.979 | 1.00 31.88 |
| ATOM | 4519 | С | | 90 | 58,505 | -5.613 | 85.085 | 1.00 21.28 |
| | | | | | | | | |
| _ATOM | 4520 | 0 | | 90 | 57.695 | -4.897 | 84.501 | 1.00 15.72 |
| ATOM | 4521 | N | - HIS B 1 | 91 | 58.857 | -5.421 | 86.351 | 1.00 18.16 |
| ATOM | 4522 | CA | HIS B 1 | 91 | 58.249 | -4.357 | 87.145 | 1.00 17:46 |
| | 4523 | CB | | 91 | 56.759 | -4.690 | | |
| AŢOM | | | | | | | 87.369 | 1.00 16.00 |
| MOTA | 4524 | CG | | 91 - | 56.517 | -6.085 | 87.880 | 1.00 22.14 |
| ATOM | 4525 | CD2 | HIS B 1 | 91 | 56.341 | -6.551 | 89.143 | 1.00 12.25 |
| ATOM | 4526 | ND1 | HIS B 1 | 91 | 56.372 | -7.179 | 87.049 | 1.00 18.02 |
| | 4527 | CE1 | | | 56.119 | -8.256 | | |
| MOTA | | | | | | | 87.775 | 1.00 8.17 |
| ATOM | 4528 | NE2 | | | 56.094 | -7.902 | 89.049 | 1.00 19.79 |
| ATOM | 4529 | С | HIS B 1 | 91 . | 58.945 | -4.197 | 88.484 | 1.00 17.41 |
| ATOM | 4530 | 0 | HIS B 1 | 91 | 59.769 | -5.029 | 88.867 | 1.00 18.74 |
| | | N | GLN B 1 | | | | | |
| MOTA | 4531 | | | | 58.618 | -3.114 | 89.182 | 1.00 18.20 |
| MOTA | 4532 | CA | GLN B 1 | 92 | 59.173 | -2.854 | 90.502 | 1.00 18.41 |
| ATOM | 4533 | CB | GLN B 1 | 92 | 58.690 | -1.500 | 91.034 | 1.00 20.71 |
| ATOM | 4534 | CG | GLN B 1 | | 58.871 | -0.334 | 90.072 | 1.00 21.49 |
| | | | | | | | | |
| ATOM | 4535 | CD | GLN B 1 | | 58.226 | 0.930 | 90.594 | 1.00 20.65 |
| ATOM | 4536 | OE1 | GLN B 19 | 92 | 58.775 | 1.615 | 91.459 | 1.00 21.52 |
| ATOM | 4537 | NE2 | GLN B 19 | 92 | 57.029 | 1.226 | 90.098 | 1.00 15.10 |
| ATOM | 4538 | С | GLN B 1 | | 58.608 | -3.945 | 91.395 | 1.00 17.55 |
| | | | | | | | | |
| ATOM | 4539 | 0 | GLN B 19 | | 57.415 | -4.256 | 91.320 | 1.00 17.48 |
| ATOM | 4540 | N | SER B 19 | | 59.447 | -4.522 | 92.240 | 1.00 15.71 |
| ATOM | 4541 | CA | SER B 19 | 93 | 58.986 | -5.574 | 93.143 | 1.00 20.58 |
| MOTA | 4542 | CB | SER B 19 | | 60.093 | -5.963 | 94.120 | 1.00 20.71 |
| | | | | | | | | |
| MOTA | 4543 | OG | SER B 19 | | 59.571 | -6.804 | 95.138 | 1.00 22.55 |
| ATOM | 4544 | С | SER B 19 | 3 | 57.774 | -5.112 | 93.947 | 1.00 21.81 |
| ATOM · | 4545 | 0 | SER B 19 | 13 | 57.769 | -4:003 | 94.486 | 1.00 20.82 |
| ATOM | 4546 | N | PRO B 19 | | 56.745 | -5.967 | 94.063 | 1.00 21.80 |
| | | | | | | | • | |
| ATOM | 4547 | CD | PRO B 19 | | 56.648 | -7.331 | 93.524 | 1.00 24.27 |
| ATOM | 4548 | CA | PRO B 19 | 14 | 55.524 | -5.643 | 94.812 | 1.00 23.58 |
| MOTA | 4549 | CB | PRO B 19 | 4 | 54.678 | -6.909 | 94.642 | 1.00 22.98 |
| ATOM | 4550 | CG | PRO B 19 | 4 | 55.168 | -7.458 | 93.317 | 1.00 26.35 |
| | 4551 | c | PRO B 19 | | 55.841 | -5.366 | 96.283 | |
| MOTA. | | | | | | | | 1.00 25.79 |
| MOTA | 4552 | ၁ | PRO B 19 | | 55.009 | -4.831 | 97.022 | 1.00 27.26 |
| MOTA | 4553 | N | GLU B 19 | 5 | 57.045 | -5.736 | 96.710 | 1.00 23.20 |
| ATOM | 4554 | CA | GLU B 19 | 5 | 57.428 | -5.514 | 98.093 | 1.00 29.56 |
| | 4555 | CB | GLU B 19 | | 58.816 | -6.090 | 98.379 | 1.00 32.38 |
| ATOM | | | | | | | | |
| ATOM | 4556 | CG | GLU B 19 | | 58.940 | -7.567 | | 1.00 45.25 |
| ATOM | 4557 | CD | GLU B 19 | 5 | 60.206 | -8.189 | 98.613 | 1.00 50.44 |
| ATOM | 4558 | OE1 | GLU B 19 | 5 | 61.290 | -7.580 | 98.471 | 1.00 50.51 |
| | 4559 | OE2 | GLU B 19 | | 60.118 | -9.297 | 99.184 | .00 49.77 |
| MOTA | | | | | | | | |
| ATOM | 4560 | C | GLU B 19 | | 57.414 | -4.035 | 98.425 | 1.00 25.11 |
| ATOM | 4561 | 0 | GLU B 19 | 5 | 57.095 | -3.659 | 99.551 | 1.00 29.05 |
| ATOM | 4562 | N | TYR B 19 | 6 | 57.729 | -3.191 | 97.445 | 1.00 22.90 |
| | 4563 | CA | TYR B 19 | | | -1.750 | 97.696 | 1.00 22.46 |
| ATOM | | | | | | | | |
| ATCM | 4564 | CB | TYR B 19 | | 59.188 | -1.223 | 97.668 | 1.00 22.72 |
| ATOM | .4565 | CG | TYR B 19 | 6 | 59.855 | -1.234 | 96.301 | 1.00 24.17 |
| ATOM | 4566 | | TYR B 19 | | 59.639 | -0.203 | 95.385 | 1.00 20.87 |
| | | | | | | | | |
| MOTA | 4567 | CE1 | TYR B 19 | | 60.229 | -0.222 | 94.118 | 1.00 18.31 |
| ATOM | 4568 | CD2 | TYR B 19 | | 60.684 | -2.289 | 95.916 | 1.00 24.63 |
| ATOM | 4569 | CE2 | TYR B 19 | 6 | 61.276 | -2.318 | 94.648 | 1.00 24.39 |
| | 4570 | | TYR B 19 | | 61.042 | -1.284 | 93.756 | 1.00 23.01 |
| MOTA | | | | | | | | |
| atom | 4571 | OH | TYR B 19 | | 61.592 | -1.328 | 92.492 | 1.00 19.86 |
| ATOM | 4572 | С | TYR B 19 | 5 | 56.896 | -0.938 | 96.725 | 1.00 23.54 |
| ATOM | 4573 | 0 | TYR B 19 | 5 | 56.779 | 0.275 | 96.869 | 1.00 17.53 |
| | 4574 | | ALA B 19 | | 56.293 | -1.589 | 95.740 | 1.00 22.11 |
| ATOM | | | | | | | | |
| ATOM | 4575 | | ALA B 19. | | 55.503 | -0.829 | 94.779 | 1.00 24.28 |
| MOTA | 4576 | | YTY B 18. | | 56.310 | -0.616 | 93.513 | 1.00 23.03 |
| | 1577 | | ALA B 19 | | 54.153 | -1.412 | 94.413 | 1.00 22.80 |
| ATOM | | | | | 34.470 | 1.414 | | |

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Figure 18-70

| ATOM | 4578 | 3 0 | ALA B | 197 | 53.91 | 0 -2.609 | 94.549 | 1.00 17,67 |
|--------------|--------------|-----------|----------------|-------|------------------|----------|------------------|--------------------------|
| ATOM | 4579 | | PHE B | 198 | 53.27 | | | |
| ATOM | 4580 | | | | 51.95 | | | 1.00 28.19 |
| ATOM | 4581 | | | | 51.15 | | 93.035 | 1.00 29.51 |
| ATOM | 4582 | CG | PHE B | 198 | 49.72 | | | 1.00 29,50 |
| MOTA | 4583 | CD | 1 PHE B | 198 | 48.73 | | 93.674 | 1.00 32.77 |
| ATOM | 4584 | CD. | 2 PHE B | 198 | 49.36 | | 91.455 | 1.00 25.82 |
| MOTA | 4585 | CE | 1 PHE B | 198 | 47.41 | | 93.394 | 1.00 36.70 |
| MOTA | 4586 | CE | 2 PHE B | .198 | 48.05 | | 91.170 | 1.00 29.29 |
| MOTA | 4587 | CZ | PHE B | 198 | 47.07 | | 92.141 | 1.00 33.05 |
| MOTA | 4588 | С | PHE B | 198 | 52.17 | | 92.284 | 1.00 28.28 |
| ATOM | 4589 | 0 | PHE B | 198 | 53.04 | | 91.456 | 1.00 27.15 |
| MOTA | 4590 | N | PRO B | 199 | 51.40 | 7 -2.952 | 92.185 | 1.00 31.37 |
| MOTA | 4591 | CD | PRO B | 199 | 51.44 | -3.887 | 91.045 | 1.00 37.07 |
| ATOM | 4592 | CA | PRO B | 199 | 50.38 | | 93.144 | |
| MOTA | 4593 | ÇВ | PRO B | 199 | 49.54 | 5 -4.328 | 92.321 | 1.00 33.88 |
| MOTA | 4594 | CG | PRO B | 199 | 50.641 | -5.068 | 91.578 | 1.00 36.75 |
| MOTA | 4595 | С | PRO B | 199 | 51.241 | 4.082 | 94.184 | 1.00 36.93 |
| ATOM | 4596 | 0 | PRO B | 199 | 52.308 | 3 -4.603 | 93.860 | 1.00 50.93 |
| MOTA | 45,97 | N | PHE B | 200 | 50.804 | 4 -4.127 | 95.422 | 1.00 37.04 |
| MOTA | 4598 | CA | PHE B | | 51.644 | 4.763 | 96.421 | 1.00 30.13 |
| ATOM | 4599 | CB | PHE B | 200 | 51.547 | -3.968 | 97.723 | 1.00 28.70 |
| MOTA | 4600 | CG | PHE B | 200 | 51.760 | -2.485 | 97.543 | 1.00 29.98 |
| MOTA | 4601 | | | 200 | 50.717 | | 97.137 | 1.00 28.92 |
| ATOM | 4602 | CD2 | | | 53.016 | | 97.746 | 1.00 23.60 |
| MOTA | 4603 | CE1 | | | 50.922 | | 96.938 | 1.00 27.63 |
| MOTA | 4604 | CE2 | | | 53.229 | | 97.547 | 1.00 23.56 |
| MOTA | 4605 | CZ | PHE B | | 52.182 | | 97.143 | 1.00 28.37 |
| ATOM | 4606 | C | PHE B | | 51.296 | | 96.658 | 1.00 25.51 |
| MOTA | 4607 | 0 | PHE B | | 52.112 | | 97.167 | 1.00 20.92 |
| ATOM | 4608 | N | GLU B | | 50.094 | | 96.252 | 1.00 27.41 |
| ATOM | 4609 | CA | GLU B | | 49.576 | | 96.454 | 1.00 31.98 |
| MOTA | 4610 | CB | GLU B | | 48.056 | | 96.487 | 1.00 31.57 |
| ATOM | 4611 | CG | GLU B | | 47.486 | | 97.449 | 1.00 39.17 |
| MOTA | 4612 | CD OE1 | GLU B GLU B | | 45.987 | | 97.316 | 1.00 40.31 |
| ATOM | 4613 4614 | OE2 | | | 45.332 45.475 | | 97.500 | 1.00 38.90 |
| ATOM ATOM | 4615 | C | | 201 | 49.979 | | 97.019 95.422 | 1.00 35.04 |
| ATOM | 4616 | Ö | | 201 | | -10.219 | 95.690 | 1.00 30.83 1.00 26.34 |
| ATOM | 4617 | N | | 202 | 50.362 | | 94.234 | 1.00 24.95 |
| ATOM | 4618 | CA | | 202 | 50.764 | | 93.195 | 1.00 22.79 |
| ATOM | 4619 | CB | | 202 | 49.588 | -9.773 | 92.258 | 1.00 25.12 |
| ATOM | 4620 | CG | | 202 | | -10.523 | 93.000 | 1.00 35.38 |
| MOTA | 4621 | CD | | 202 | | -11.099 | 92.103 | 1.00 38.67 |
| ATOM | 4622 | CE | LYS B | | | -11.998 | 92.903 | 1.00 40.98 |
| ATOM | 4623 | NZ | LYS B | | | -12.659 | 92.028 | 1.00 46.65 |
| ATOM | 4624 | С | LYS B : | | 51.975 | -9.007 | 92.435 | 1.00 24.62 |
| MOTA | 4625 | 0 | LYS B 2 | 202 | 52.355 | -7.838 | 92.549 | 1.00 21.83 |
| MOTA | 4626 | N | GLY B 2 | 203 | 52.598 | -9.910 | 91.684 | 1.00 17.60 |
| ATOM | 4627 | CA | GLY B 2 | 203 | 53.779 | -9.545 | 90.928 | 1.00 19.41 |
| ATOM | 4628 | С | GLY B 2 | 203 | | -10.297 | 91.396 | 1.00 20.36 |
| ATOM | 4629 | 0 | GLY B 2 | 203 | 56.101 | -10.070 | 90.888 | 1.00 23.83 |
| ATOM | 4630 | N | PHE B 2 | 204 | 54.855 | -11.201 | 92.358 | 1.00 24.82 |
| MOTA | 4631 | CA | PHE B 2 | | | ~11.957 | 92.859 | 1.00 24.24 |
| ATOM | 4632 | CB | PHE B 2 | | 55.690 | -12.567 | 94.236 | 1.00 22.72 |
| ATOM | 4633 | CG | PHE B 2 | | | -11.549 | 95.322 | 1.00 25.26 |
| ATOM | 4634 | CD1 | PHE B 2 | | | -10.977 | 95.535 | 1.00 23.80 |
| ATÓM | 4635 | CD2 | PHE B 2 | | | -11.159 | 96.133 | 1.00 20.25 |
| ATOM | 4636 | CEl | PHE B 2 | | | -10.036 | 96.545 | 1.00 29.98 |
| ATOM | 4637 | CE2 | PHE B 2 | | | -10.221 | 97.141 | 1.00 24.40 |
| ATOM | £638 | CE | PHE B 2 | | 55.124 | -9.658 | 97.350 | 1.00 25.54 |
| ATOM | 4639 | C | PHE B 2 | | | -13.057 | 91.894 | 1.00 25.86 |
| ATCM | 4640 | | PHE B 2 | | | -13.540 | 91.091 | 1.00 20.65 |
| MOTA | 1641 | | LEU B 2 | | 5/.676 | -13.449 | 91.986 | 1.00 24.25 |
| ATOM | 4642 | | LEU B 2 | - | 58.233 | -14.472 | 91.114 | 1.00 30.66 |
| ATOM | 4643 | | LEU B 2 | . U D | by. 723 | -14.637 | 91.413 | 1.00 34.01 |

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Figure 18-71

| MOTA | 4644 | CG LEU | Э 205 | 60.49 | 5 -15.669 | 90.592 | 1.00 | 34.12 |
|--------------|--------------|----------------|----------------|------------------|------------------------|------------------|------|-----------------------------|
| ATOM | 4645 | CD1 LEU | | | 5 -15.382 | 89.109 | 1.00 | 32.95 |
| MOTA | 4646 | CD2 LEU | | | 7 -15.629 | 91.005 | | 36.49 |
| MOTA | 4647 | C LEU | | | -15.827 | 91.205 | | 30.51 |
| ATOM ATOM | 4648 4649 | O LEU N GLU | | | 7 -16.562 9 -16.147 | 90.220 | | 25.89 |
| ATOM | 4650 | CA GLU | | 56.338 | | 92.382 92.605 | | 30.43 30.64 |
| ATOM | 4651 | CB GLU | | 56.025 | | 94.093 | | 34.77 |
| ATOM | 4652 | CG GLU | | 57.227 | -17.512 | 95.033 | | 42.50 |
| ATOM | 4653 | CD GLU | B 206 | 57.718 | | 95.270 | | 45.76 |
| ATOM | 4654 | OE1 GLU | B 206 | 58.228 | -15.438 | 94.333 | | 42.62 |
| ATOM | 4655 | | B 206 | 57.585 | | 96.413 | 1.00 | 50.22 |
| MOTA | 4656 | | Э 206 | | -17.587 | 91.811 | | 31.13 |
| MOTA | 4657 | | B 206 | | -18.708 | 91.563 | | 28.18 |
| MOTA | 4658 | | B 207 B 207 | | -16.472 | 91.425 | | 25.16 |
| MOTA MOTA | 4659 4660 | | B 207 | | -16.499 -15.107 | 90.664 90.695 | | 28.78 30.76 |
| ATOM | 4661 | CG GLU | | 52.121 | -14.659 | 92.093 | | 29.39 |
| ATOM | 4662 | CD GLU | | | -13.151 | 92.230 | | 27.87 |
| ATOM | 4663 | OE1 GLU | | | -12.477 | 91.261 | | 24.38 |
| ATOM | 4664 | OE2 GLU | B 207 | 52.389 | -12.636 | 93.316 | | 25.36 |
| MOTA | 4665 | C GLU | в 207 . | 53.453 | -16.922 | 89.224 | 1.00 | 29.48 |
| MOTA | 4666 | o GLU | | 53.658 | | 88.351 | | 27.48 |
| MOTA | 4667 | | B 208 | | -18.230 | 88.976 | | 26.67 |
| ATOM | 4668 | CA ILE | | 53.735 | | 87.646 | | 32.60 |
| ATOM | 4669 4670 | CB ILE : | | 54.789 55.239 | | 87.740 86.352 | | 34.26 |
| ATOM ATOM | 4671 | CG1 ILE | | 56.008 | | 88.532 | | 41.65 36.07 |
| ATOM | 4672 | CD1 ILE | | 56.814 | | 87.851 | | 45.18 |
| ATOM | 4673 | C ILE | | 52.522 | -19.289 | 86.870 | | 32.26 |
| ATOM | 4674 | O ILE | B 208 | | -19.799 | 85.759 | | 27.43 |
| ATOM | 4675 | N GLY | | 51.328 | -19.165 | 87.442 | 1.00 | 32.60 |
| MOTA | 4676 | CA GLY I | | 50.139 | | 86.760 | | 35.07 |
| ATOM | 4677 | C GLY | | 49.565 | -20.892 | 87.420 | | 36.19 |
| ATOM | 4678 4679 | O GLY I | | 50.230 | -21.524 | 88.235 | | 31.61 |
| ATOM ATOM | 4680 | N GLU I | | | -21.245 -22.412 | 87.066 87.647 | | 36.98 |
| ATOM | 4681 | CB GLU B | | | -21.964 | 88.672 | | 37.98 |
| ATOM | 4682 | CG GLU | | | -21.234 | 88.058 | | 42.78 |
| ATOM | 4683 | CD GLU | 3 210 | | -20.717 | 89.098 | | 48.41 |
| ATOM | 4684 | OE1 GLU | 3 210 | 43.400 | -20.202 | 88.709 | 1.00 | 51.03 |
| ATOM | 4685 | OE2 GLU F | | 44.778 | -20.814 | 90.306 | | 49.90 |
| ATOM | 4686 | C GLU E | | | -23.248 | 86.564 | | 39.48 |
| ATOM | 4687 | O GLU E | | | -22.751 | 85.471 | | 33.65 |
| ATOM ATOM | 4688 4689 | N GLY E | | | -24.515 -25.399 | 86.876 85.923 | | 39.18 38.43 |
| ATOM | 4690 | | 211 | | -25.500 | 84.637 | | 40.29 |
| ATOM | 4691 | | 211 | 48.101 | -25.610 | 84.666 | | 39.39 |
| ATOM | 4692 | N LYS B | | | -25.458 | 83.504 | | 40.90 |
| MOTA | 4693 | CA LYS B | 212 | 46.864 | -25.538 | 82.219 | 1.00 | 43.53 |
| ATOM | 4694 | CB LYS B | | | -25.548 | 81.080 | | 47.87 |
| ATOM | 4695 | CG LYS B | | | -26.665 | 81.144 | | 53.09 |
| ATOM | 4696 | CD LYS B | | | -28.076 | 81.130 | | 58.61 |
| ATOM | 4697 | CE LYS B | | | -28.454 | 82.452 | | 59.78 |
| ATOM ATOM | 4698 4699 | NZ LYS B | | | -29.825 -24.363 | 82.420 82.040 | | 62.17 38.84 ⁻ |
| ATOM | 4700 | O LYS B | 212 | | -24.457 | 81.295 | | 40.33 |
| ATOM | 4701 | N GLY B | | 47.543 | -23.262 | 82.731 | | 37.20 |
| ATOM | 4702 | CA GLY B | | | -22.081 | 82.627 | | 34.66 |
| ATOM | 4703 | C GLY B | 213 | | -22.107 | 83.505 | | 37.09 |
| ATOM | 4704 | O GLY B | | 50.425 | -21.165 | 83.489 | | 25.85 |
| ATOM | 4705 | N LYS B | | | -23.180 | 84.273 | | 33.33 |
| MOTA | 4706 | CA LYS B | | | -23.297 | 85.148 | 1.00 | |
| ATOM | 1707 | CB LYS B | | | -24.598 | 85.954 | 1.00 | |
| ATOM | 4708 | CG LYS B | | 52.032 | -24.786 | 86.938 87.704 | 1.00 | |
| atom | 4709 | CD LYS B | 4 T A | 27.8/6 | -26.094 | 01.104 | 1.00 | 42.0U |

| ATOM | 4710 | CE | LYS B | 214 | 53.047 | -26.334 | 88.640 | 1.00 47.36 |
|--------------|--------------|----------|---------|-----|------------------|----------------------|------------------|--------------------------|
| MOTA | 4711 | NZ | LYS B | 214 | 53.165 | -25.264 | 89.666 | 1.00 54.03 |
| MOTA | 4712 | С | LYS B | 214 | 52.209 | ~23.275 | 84.291 | 1.00 34.16 |
| ATOM | 4713 | 0 | LYS B | 214 | 52.404 | -24.136 | 83.438 | 1.00 34.70 |
| MOTA | 4714 | 14 | GLY B | 215 | 53.057 | -22.279 | 84.523 | 1.00 33.58 |
| MOTA | 4715 | CA | GLY B | | 54.275 | -22.152 | 83.743 | 1.00 28.27 |
| MOTA | 4716 | C | GLY B | | 54.104 | -21.155 | 82.605 | 1.00 31.02 |
| MOTA | 4717 | 0 | GLY B | | 55.033 | -20.911 | 81.833 | 1.00 23.68 |
| MOTA | 4718 | N | TYR B | | | -20.564 | 82.493 | 1.00 22.45 |
| MOTA | 4719 | CA | TYR B | | | -19.605 | 81.426 | 1.00 24.03 |
| MOTA | 4720 | CB | TYR B | | | -20.013 | 80.603 | 1.00 17.60 |
| MOTA | 4721 | CG | TYR B | | | -21.291 | 79.806 | 1.00 25.96 |
| MOTA | 4722 | | TYR B | | | -22.538 | 80.435 | 1.00 21.41 |
| MOTA | 4723 4724 | CE1 | | 216 | | -23.704 | 79.729 78.439 | 1.00 23.78 1.00 19.62 |
| MOTA | 4725 | CD2 | | 216 | | -21.242 -22.402 | 77.722 | 1.00 19.82 |
| MOTA | 4726 | CZ | | 216 | | -23.630 | 78.379 | 1.00 29.35 |
| MOTA MOTA | 4727 | ОН | TYR B | | | -24.782 | 77.690 | 1.00 27.75 |
| ATOM | 4728 | C. | TYR B | | | -18.153 | 81.884 | 1.00 24.53 |
| ATOM | 4729 | 0 | | 216 | | -17.298 | 81.159 | 1.00 18.99 |
| ATOM | 4730 | N | ASN B | | | -17.886 | 83.098 | 1.00 21.41 |
| ATOM | 4731 | CA | ASN B | | | -16.534 | 83.642 | 1.00 21.23 |
| ATOM | 4732 | CB | ASN B | 217 | 51.954 | -16.325 | 84.669 | 1.00 16.78 |
| MOTA | 4733 | CG | ASN B. | 217 | 51.882 | -14.889 | 85.162 | 1.00 22.07 |
| MOTA | 4734 | | ASN B | | | -14.521 | 86.163 | 1.00 23.13 |
| ATOM | 4735 | | asn b | | | -14.058 | 84.435 | 1.00 19.26 |
| MOTA | 4736 | С | ASN B | | | -16.339 | 84.291 | 1.00 19.40 |
| ATOM | 4737 | 0 | ASN B | | | -17.145 | 85.124 | 1.00 19.28 |
| MOTA | 4738 | N | LEU B | | | -15.273 | 83.905 | |
| MOTA | 4739 4740 | CA CB | LEU B | | | -15.004 -15.244 | 84.444 83.368 | 1.00 16.41 1.00 18.29 |
| ATOM | 4741 | CG | LEU B | | | -15.872 | 83.782 | 1.00 18.29 |
| ATOM ATOM | 4742 | | LEU B | | | -15.563 | | 1.00 20.50 |
| ATOM | 4743 | | LEU B | | | -15.348 | | 1.00 22.53 |
| MOTA | 4744 | C | LEU B | | | -13.562 | 84.926 | 1.00 17.89 |
| ATOM | 4745 | 0 | LEU B | | | -12.627 | 84.128 | 1.00 14.48 |
| ATOM | 4746 | N | ASN B | 219 | 56.859 | -13.395 | 86.219 | 1.00 14.09 |
| MOTA | 4747 | CA | ASN B | 219 | 57.044 | -12.075 | 86.821 | 1.00 18.41 |
| MOTA | 4748 | CB | ASN B | | | -11.922 | 88.111 | 1.00 14.64 |
| MOTA | 4749 | CG | ASN B | | | -11.898 | 87.868 | 1.00 27.12 |
| MOTA | 4750 | | ASN B | | | -11.332 | 86.880 | 1.00 20.21 |
| ATOM | 4751 | | ASN B | | | -12.480 | 88.787 | 1.00 23.62 |
| MOTA | 4752 | C | ASN B | | | -11.843 | 87.172 | 1.00 20.39 |
| MOTA | 4753 | N O | ASN B | | | -12.672 -10.717 | 87.841 86.729 | 1.00 20.41 |
| MOTA MOTA | 4754 4755 | CA | ILE B. | | | -10.717 | 87.033 | 1.00 17.16 |
| ATOM | 4756 | CB | ILE B | | | -10.083 | 85.740 | 1.00 20.78 |
| ATOM | 4757 | CG2 | ILE B | | 62.736 | -9.821 | 86.094 | 1.00 18.08 |
| MOTA | 4758 | CG1 | ILE B 2 | | | -11.250 | 84.748 | 1.00 17.62 |
| MOTA | 4759 | CD1 | ILE B 2 | | | -12.590 | 85.273 | 1.00 20.72 |
| ATOM | 4760 | С | ILE B 2 | 220 | 60.475 | -9.161 | 87.947 | 1.00 21.17 |
| ATOM | 4761 | 0 | ILE B 2 | 220 | 60.565 | -8.036 | 87.470 | .1.00 16.03 |
| ATOM | 4762 | N | PRO B 2 | 221 | 60.367 | -9.357 | 89.274 | 1.00 21.74 |
| MOTA | 4763 | CD | PRO B 2 | 221 | | -10.619 [°] | 90.000 | 1.00 22.96 |
| ATOM | 4764 | CA | PRO B 2 | | 60.394 | -8.225 | 90.213 | 1.00 19.16 |
| MOTA | 4765 | CB | PRO B 2 | | 59.947 | -8.869 | 91.523 | 1.00 19.40 |
| ATOM | 4766 | CG | PRO B 2 | | | -10.251 | 91.407 | 1.00 23.02 |
| MOTA | 4767 | C | PRO B 2 | | 61.799 | -7.634 | 90.289 | 1.00 22.42 |
| MOTA | 4768 | 0 | PRO B 2 | | .62.780 | -8.369 | 90.425 90.202 | 1.00 20.71 |
| ATOM | 4769 | И | LEU B 2 | | 61.899 | -6.309 | 90.202 | 1.00 22.74 1.00 21.18 |
| ATOM | 4770 | CA | LEU B 2 | | 63.198 63.453 | -5.643 -4.993 | 88.850 | 1.00 21.18 |
| ATOM | 4771 | CB | LEU B 2 | | 63.467 | -4.993 -6.027 | 87.721 | 1.00 17.21 |
| ATOM | 4772 | CG | LEU B 2 | | 63.453 | -5.354 | 86.361 | 1.00 20.00 |
| ATOM | 4773 4774 | CD3 | LEU B 2 | 22 | 64.696 | -6.908 | 87.881 | 1.00 21.93 |
| | 4775 | CDZ | LEU B 2 | | 63.335 | -4.616 | 91.353 | 1.00 20.04 |
| ATOM | 4 | - | | | | 2.020 | | |

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```
ATOM
        4776
               0
                   LEU B 222
                                    62.350
                                             -4.030
                                                      91.806
                                                               1.00 17.58
                   PRO B 223
                                    64.571
                                             -4.394
                                                      91.830 . 1.00 19.48
ATOM
        4777
                                                      91.400
               CD
                   PRO B 223
                                    65.806
                                             ~5.072
                                                               1.00 16.80
MOTA
        4778
ATOM
        4779
               CA
                   PRO B 223
                                    64.873
                                             -3.454
                                                      92.915
                                                               1.00
                                                                    20.38
        4780
               CB
                   PRO B 223
                                    66.274
                                             -3.881
                                                      93.327
ATOM
                                                               1.00 26.11
               CG
                   PRO B 223
                                    66.884
                                             -4.161
MOTA
        4781
                                                      91.973
                                                               1.00 19.74
                   PRO B 223
                                    64.818
                                             -1.971
                                                      92.553
MOTA
        4782
               C
                                                               1.00 21.39
        4783
               O
                   PRO B 223
                                    64.815
                                             -1.598
                                                      91.380
                                                               1.00 17.16
ATOM
ATOM
        4784
               N
                   LYS B 224
                                    64.798
                                             -1.142
                                                      93.589
                                                               1.00 20.65
                   LYS B 224
                                    64.755
        4785
               CA.
                                              0.311
                                                      93.462
                                                               1.00 27.00
MOTA
                                    64.577
                                              0.938
                                                      94.844
        4786
               CB
                   LYS B 224
MOTA
                                                               1.00
                                                                    36:47
                                                     95.651
97.101
        4787
               CG
                   LYS .B 224
                                    63.415
                                              0.389
                                                               1.00 37.72
ATOM
ATOM
        4788
               CD
                   LYS B 224
                                    63.541
                                              0.833
                                                               1.00 42.06
        4789
               CE
                                    62.420
                                              0.276
                                                      97.955
ATOM
                   LYS B 224
                                                               1.00 45.18
        4790
                   LYS B 224
                                    62.645
                                              0.570
                                                      99.399
MOTA
               NZ
                                                               1.00 46.30
                                                               1.00 27.01
        4791
               C
                   LYS B 224
                                    66.071
                                              0.808
                                                      92.874
ATOM
ATOM
        4792
              0
                   LYS B 224
                                    67.098
                                              0.139
                                                      92.995
                                                               1.00 21.54
        4793
                   GLY B 225
                                    66.038
                                              1.989
                                                      92.259
                                                               1.00 22.66
MOTA
                   GLY B 225
                                    67.239
                                              2.565
                                                      91.669
        4794
              CA
                                                               1.00 25.67
ATOM
        4795
              C
                   GLY B 225
                                    67.768
                                              1.809
                                                      90.459
                                                               1.00
                                                                    24.95
ATOM
                   GLY B 225
                                    68.917
                                              1.975
                                                      90.069
                                                               1.00 26.83
ATOM
        4796
              Ö
                                                               1.00 21.79
                   LEU B 226
                                    66.926
                                              0.980
                                                     89.855
ATOM
        4797
              N
ATOM
        4798
              CA
                   LEU B 226
                                    67.319
                                              0.180
                                                      88.692
                                                               1.00
                                                                    22.91
        4799
              CB
                   LEU B 226
                                    66.067
                                             -0.473
                                                      88.099
                                                               1.00 23.29
ATOM
        4800
              CG
                   LEU B 226
                                    66.238
                                            -1.605
                                                      87.091
                                                               1.00
                                                                    26.71
ATOM
                   LEU B 226
                                    66.846
                                            -2.804
                                                      87.813
                                                               1.00 26.44
MOTA
        4801
              CD1
        4802
              CD2:LEU B 226
                                    64.877
                                            -1.997
                                                      86.508
                                                               1.00 22.96
ATOM
                   LEU B 226
                                    68.008
                                              1.017
                                                      87.603
                                                               1.00
        4803
              C
                                                                    22.66
ATOM
                   LEU B 226
                                    67.517
                                              2.087
                                                     87.250
                                                               1.00 20.19
ATOM
        4804
              0
                   ASN B 227
                                              0.549
                                                     87,060
                                                               1.00 15.52
ATOM
        4805
              N
                                    69.134
        4806
              CA
                   ASN B 227
                                    69.794
                                              1.317
                                                     85.998
                                                               1.00
                                                                    19.49
ATOM
                                                               1.00 20.43
                   ASN B 227
                                                     86.270
        4807
              CB
                                    71.304
                                             1.474
ATOM
                                    72.062
                                                     86.206
                   ASN B 227
                                                               1.00 28.97
        4808
              CG
                                              0.161
ATOM
                                                               1.00 24.30
                                                     85.199
MOTA
        4809
              OD1
                  ASN B 227
                                    72.015
                                            -0.546
                  ASN B 227
                                    72.786
                                            -0.1,60
                                                     87.276
                                                               1.00 20.88
ATOM
        4810
ATOM
        4811
                   ASN B 227
                                    69.548
                                             0.671
                                                     84.630
                                                               1.00 21.26
              C
                                                               1.00 18.90
                                    69.004
                                            -0.432
                                                     84.555
ATOM
        4812
              0
                   ASN B
                         227
                   ASP B 228
                                    69.949
                                             1.347
                                                     83.552
                                                               1.00 20.98
MOTA
        4813
              Ν
                                    69.720
                                                     82.208
                                                               1.00
                                                                    22.61
ATOM
        4814
              CA
                  ASP
                       В
                         228
                                             0.817
                  ASP B 228
                                    70.270
                                             1.753
                                                     31.126
                                                               1.00 23.46
              CB
ATOM
        4815
ATOM
                                    69.596
                                                               1.00 26.12
        4816
              CG
                   ASP 3 228
                                             3.113
                                                     81,119
                                    68.387
                                                     81.415
                                                               1.00 26.75
ATOM
        4817
              OD1
                  ASP
                       В
                         .228
                                             3.193
        1818
              OD2
                  ASP B 228
                                   70.276
                                              4.101
                                                     80.773
                                                               1.00 30.22
ATOM
                                            -0.573
                                                     81.952
                                                               1.00 23.49
                                   70.286
ATOM:
        4819
              C
                   ASP B 228
        4820
              0
                   ASP B
                         228
                                   69.651
                                            -1.390
                                                     81,288
                                                               1.00 19.31
ATOM
       4821
              N
                  ASN B 229
                                   71.484
                                            -0.836
                                                     82.453
                                                               1.00 22.24
ATCM
                                                     82.250
                                                               1.00 23.30
                  ASN B 229
                                   72.111
                                            -2.135
ATOM
       4822
              CA
                                                     82,737
ATOM
       4823
              CB
                  ASN B 229
                                   73.562
                                            -2.101
                                                               1.00 20.99
       4824
                  ASN B 229
                                   74.441
                                            -1.237
                                                     81.859
                                                               1.00 25.71
              CG
ATOM
                                                     80.678
                                   74.644
                                                               1.00 26.40
                  ASN B 229
                                            -1.538
STOM
       4825
              OD1
                                                               1.00 27.44
ATOM
       4826
              ND2
                  ASN B
                         229
                                   74.955
                                            -0.151
                                                     82.417
                                                               1.00 23.74
       4827
                  ASN B 229
                                   71.341
                                            -3.252
                                                     82,943
              C
ATCM
                                                     82.402
                                   71.207
                                                               1.00 20.51
                  ASN B 229
                                            -4.346
MOTA
       1828
              0
       4829
              N
                  GLU B 230
                                   70.832
                                            -2.976
                                                     84.139
                                                               1.00 23.06
ATOM
                  GLU B 230
                                   70.069
                                            -3.977
                                                     84.874
                                                               1.00 23.01
       4830
              CA
ATOM
                                                     86.297
                                   69.799
                                            -3.480
                                                               1.00 24.73
              CB
                  GLU 3 230
ATOM
       4831
                                                     87.087
MOTA
       4832
              CG
                  GLU B
                         230
                                   71.069
                                            -3.201
                                                               1.00 27.28
                                                     88.470
                                                               1.00 27.47
       4833
              CD
                  GLU B 230
                                   70.792
                                            -2.649
ATOM
                                                               1.00 27.87
                                                     88.569
                                   70.086
                  GLU B 230
                                            -1.625
ATOM
       4834
             OE1
                                                     89.455
                                                               1.00 26.79
       1835
              OE2
                  GLU B 230
                                   71.286
                                            ~3.232
ATOM
                                                               1.00 24.25
                  GLU B 230
                                   68.749
                                            -4.281
                                                     84.146
ATOM
       1836
             С
                                                               1.00 15.89
                                                     84.022
                  GLU B 230
                                   68.347
                                            -5.445
       4837
             0
ATOM
                                                               1.00 21.46
       :838
             N
                  PHE B
                         231
                                   68.091
                                            -3.242
                                                     83.637
ATCM
                                            -3.429
                                                     82.933
                                                               1.00 22.84
                  PHE B 231
                                   66.814
             CA
       4839
ATOM
                                                               1.00 23.96
                  PHE B 231
                                            -2.079
                                                     82.529
       4840
                                   66.210
             CB
atom
                  PHE B 231
                                   64.803
                                                     81.975
                                                               1.00 26.13
       4841
             CG
                                            -2.182
ATOM
```

| > moM | 4842 | CD1 | .PHE B | 221 | | 63.738 | -2.514 | 82.805 | 1.00 25.00 |
|-------|------|-----|--------|-----|-----|--------|---------|----------------------|------------|
| MOTA | | | PHE B | | | 64.550 | -1.956 | 80.627 | 1.00 22.93 |
| MOTA | 4843 | CD2 | | | | | | 82.304 | 1.00 25.03 |
| MOTA | 4844 | CE1 | | | | 62.440 | -2.618 | | |
| MOTA | 4845 | CE2 | PHE B | | | 63.250 | -2.059 | 80.114 | 1.00 27.46 |
| MOTA | 4846 | cz | PHE B | 231 | | 62.196 | -2.390 | 80.957 | 1.00 20.25 |
| MOTA | 4847 | С | PHE B | 231 | | 66.978 | -4.288 | 81.677 | 1.00 23.14 |
| ATOM | 4848 | 0 | PHE B | 231 | | 66.221 | -5.239 | 81.464 | 1.00 20.02 |
| MOTA | 4849 | N | LEU B | 232 | | 67.963 | -3.952 | 80.845 | 1.00 22.02 |
| | 4850 | CA | LEU B | | | 68.200 | -4.697 | 79.614 | 1.00 19.97 |
| MOTA | | СВ | LEU B | | • | 69.192 | -3.942 | 78.734 | 1.00 24.99 |
| MOTA | 4851 | | | | | 68.665 | -2.581 | 78.263 | 1.00 29.73 |
| MOTA | 4852 | CG | LEU B | | | | | 77.454 | 1.00 28.11 |
| ATOM | 4853 | CD1 | | | | 69.746 | -1.856 | | |
| MOTA. | 4854 | CD2 | | | | 67.409 | -2.784 | 77.414 | 1.00 26.54 |
| MOTA | 4855 | С | LEU B | 232 | | 68.688 | -6.119 | 79.898 | 1.00 19.25 |
| ATOM | 4856 | 0 | LEU B | 232 | | 68.365 | -7.051 | 79.162 | 1.00 19.49 |
| MOTA | 4857 | N | PHE B | 233 | | 69.468 | -6.280 | 80.962 | 1.00 20.50 |
| ATOM | 4858 | CA | PHE B | 233 | | 69.950 | -7.599 | 81.378 | 1.00 20.70 |
| MOTA | 4859 | CB | PHE B | | | 70.825 | -7.471 | 82.632 | 1.00 23.75 |
| MOTA | 4860 | CG | PHE B | | | 71.217 | -8.790 | 83.239 | 1.00 28.58 |
| | 4861 | CD1 | PHE B | | | 72.285 | -9.519 | 82.731 | 1.00 30.48 |
| MOTA | 4862 | CD2 | PHE B | | | 70.481 | -9.328 | 84.294 | 1.00 25.32 |
| MOTA | | CE1 | PHE B | | | | -10.762 | 83.262 | 1.00 31.87 |
| MOTA | 4863 | | | | | 70.803 | -10.573 | 84.832 | 1.00 31.26 |
| ATOM | 4864 | CE2 | PHE B | | | 70.603 | -11.292 | 84.317 | 1.00 32.29 |
| MOTA | 4865 | CZ | PHE B | | | | | | |
| MOTA | 4866 | С | | 233 | • | 68.712 | -8.439 | 81.727 | 1.00 20.23 |
| MOTA | 4867 | 0 | PHE B | | | 68.553 | -9.567 | 81.270 | 1.00 21.56 |
| MOTA | 4868 | N | | 234 | | 67.842 | -7.878 | 82.560 | 1.00 21.26 |
| ATOM | 4869 | CA | | 234 | • . | 66.626 | -8.576 | 82.963 | 1.00 19.60 |
| ATOM | 4870 | CB | ALA B | 234 | | 65.835 | -7.733 | 83.950 | 1.00 19.25 |
| MOTA | 4871 | С | ALA B | 234 | | 65.772 | -8.898 | 81.749 | 1.00 18.87 |
| ATOM | 4872 | 0 | ALA B | 234 | | 65.253 | ~10.010 | 81.624 | 1.00 21.91 |
| ATOM | 4873 | N | LEU B | 235 | | 65.634 | -7.934 | 80.845 | 1.00 20.29 |
| ATOM | 4874 | CA | LEU B | 235 | | 64.822 | -8.141 | 79.652 | 1.00 19.53 |
| ATOM | 4875 | CB | LEU B | 235 | | 64.773 | -6:874 | 78 [.] .795 | 1.00 24.07 |
| ATOM | 4876 | CG | LEU B | 235 | | 63.465 | -6.607 | 78.024 | 1.00 27.87 |
| ATOM | 4877 | | | 235 | | 63.783 | -5.813 | 76.770 | 1.00 20.77 |
| | 4878 | | LEU B | | | 62.761 | -7.897 | 77.664 | 1.00 26.94 |
| ATOM | 4879 | c | | 235 | | 65.376 | -9.276 | 78.795 | 1.00 20.79 |
| ATOM | 4880 | 0 | LEU E | | | 64.648 | -10.205 | 78.431 | 1.00 18.25 |
| MOTA | | | GLU B | | | 66.665 | -9.191 | 78.462 | 1.00 19.33 |
| MOTA | 4881 | N | | | | 67.303 | -10.206 | 77.629 | 1.00 27.93 |
| MOTA | 4882 | CA | GLU B | | | | -9.853 | 77.384 | 1.00 31.06 |
| atom | 4883 | CB | GLU B | | | 68.777 | | 76.548 | 1.00 43.60 |
| MOTA | 4884 | CG | GLU B | 236 | | 68.969 | -8.597 | 76.259 | 1.00 45.19 |
| ATOM | 4885 | CD | | 236 | | 70.428 | -8.292 | | |
| ATOM | 4886 | OEl | | 236 | | 70.697 | -7.309 | 75.538 | 1.00 48.77 |
| ATOM | 4887 | OE2 | GLU B | 236 | | 71.300 | -9.032 | 76.751 | 1.00 52.72 |
| ATOM | 4888 | С | GLU B | 236 | | 67.20_ | -11.607 | 78.209 | 1.00 24.89 |
| ATOM | 4889 | 0 | GLU B | 236 | | 238.36 | -12.552 | 77.501 | 1.00 22.06 |
| ATOM | 4890 | N | LYS B | 237 | | 67.520 | -11.748 | 79.492 | 1.00 24.20 |
| ATOM | 4891 | CA | LYS B | 237 | | 67.449 | -13.058 | 80.130 | 1.00 27.10 |
| ATOM | 4892 | CB | LYS B | 237 | | 67.989 | -12.984 | 81.562 | 1.00 23.43 |
| MOTA | 4893 | CG | LYS B | | | | -12.641 | 81.650 | 1.00 29.46 |
| MOTA | 4894 | CD | LYS B | | | | -13.683 | 80.924 | 1.00 31.65 |
| | 4895 | CE | | 237 | | 71 782 | -13.356 | 80.993 | 1.00 39.70 |
| MOTA | | | | 237 | | | -14.363 | 80.242 | 1.00 46.74 |
| MOTA | 4896 | NZ | | | | 66.019 | -13.615 | 80.143 | 1.00 30.92 |
| MOTA | 4897 | Č | | 237 | | | | 79.763 | 1.00 31.42 |
| MOTA | 4898 | 0 | | 237 | | | -14.766 | 80.573 | 1.00 25.86 |
| ATOM | 4899 | Ŋ | | 238 | | 65.057 | -12.806 | 80.620 | 1.00 27.98 |
| MOTA | 4900 | CA | SER B | | | 63.677 | -13.280 | | 1.00 27.90 |
| MOTA | 4901 | CB | | 238 | | 62.776 | -12.241 | 81.289 | 1.00 20.03 |
| ATOM | 4902 | OG | SER B | 238 | | 62.756 | -11.028 | 80.565 | 1.00 29.27 |
| MOTA | 1903 | С | SER E | 238 | | | -13.642 | 79.229 | 1.00 28.32 |
| MOTA | 4904 | 0 | SER B | 238 | | | -14.605 | 79.089 | 1.00 29.65 |
| ATOM | 1905 | N | | 239 | | 63.536 | -12.886 | 78.203 | 1.00 27.39 |
| ATOM | 4906 | CA | LEU B | 239 | | | -13.192 | 76.846 | 1.00 32.52 |
| ATOM | 4907 | CB | LEU B | 239 | | 63.544 | -12.129 | 75.837 | 1.00 30.53 |
| | | | | | | | | - | |

| ATOM | 4908 CG LEU B 239 | 62.833 -10.772 | 75.895 | 1.00 36.06 |
|--------------|--|----------------------------------|------------------|--------------------------|
| ATOM | | 63.404 -9.836 | 74.842 | 1.00 29.64 |
| ATOM | | 61.338 -10.976 | | 1.00 30.73 |
| MOTA MOTA | | 63.598 -14.563 | | |
| ATOM | 4912 O LEU B 239 4913 N GLU B 240 | 62.879 -15.340 | | |
| ATOM | 4914 CA GLU B 240 | 64.844 ~14.859 65.434 ~16.152 | | |
| ATOM | 4915 CB GLU B 240 | 66.859 -16.238 | 77.011 | |
| ATOM | 4916 CG GLU B.240 | 67.878 -15.407 | 76.275 | 1.00 40.56 |
| ATOM | 4917 CD GLU B 240 | 69.256 -15.532 | 76.903 | 1.00 48.20 |
| ATOM | 4918 OE1 GLU B 240 | 69.685 -16.679 | 77.161 | 1.00 45.36 |
| ATOM ATOM | 4919 OE2 GLU B 240 4920 C GLU B 240 | 69.912 -14.492 | 77.130 | 1.00 48.21 |
| ATOM | 4921 O GLU B 240 | 64.604 -17.258 64.391 -18.310 | 77.108 | 1.00 33.23 |
| ATOM | 4922 N ILE B 241 | 64.146 -17.017 | 76.510 78.331 | 1.00 32.15 1.00 29.72 |
| ATOM | 4923 CA ILE B 241 | 63.328 -17.989 | 79.047 | 1.00 29.72 |
| ATOM | 4924 CB ILE B 241 | 63.006 -17.489 | 80.466 | 1.00 30.42 |
| MOTA | 4925 CG2 ILE B 241 | 62.049 -18.456 | 81.162 | 1.00 29.88 |
| ATOM ATOM | 4926 CG1 ILE B 241 4927 CD1 ILE B 241 | 64.309 -17.311 | 81.254 | 1.00 29.77 |
| ATOM | 4928 C ILE B 241 | 64.118 -16.760 62.016 -18.247 | 82.654 | 1.00 32.92 |
| ATOM | 4929 0 ILE B 241 | 61.592 -19.396 | 78.298 78.149 | 1.00 34.65 1.00 30.22 |
| ATOM | 4930 N VAL B 242 | 61.379 -17.178 | 77.823 | 1.00 30.22 |
| ATOM | 4931 CA VAL B 242 | 60.114 -17.312 | 77.105 | 1.00 34.55 |
| MOTA MOTA | 4932 CB VAL B 242 4933 CG1 VAL B 242 | 59.476 -15.937 | 76.825 | 1.00 30.77 |
| ATOM | 4933 CG1 VAL B 242 4934 CG2 VAL B 242 | 58.191 -16.113 59.201 -15.214 | 76.038 | 1.00 32.18 |
| ATOM | 4935 C VAL B 242 | 60.320 -18.042 | 78.140 75.787 | 1.00 31.57 1.00 36.56 |
| MOTA | 4936 C VAL B 242 | 59.572 -18.959 | 75.453 | 1.00 33.93 |
| MOTA | 4937 N LYS B 243 | 61.337 -17.627 | 75.042 | 1.00 38.64 |
| ATOM ATOM | 4938 CA LYS B 243 4939 CB LYS B 243 | 61.659 -18.241 | 73.760 | 1.00 44.36 |
| ATOM | 4939 CB LYS B 243 4940 CG LYS B 243 | 62.966 -17.659 62.810 -16.399 | 73.214 | 1.00 48.33 |
| ATOM | 4941 CD LYS B 243 | 62.185 -16.718 | 72.386 71.036 | 1.00 53.88 1.00 53.72 |
| ATOM | 4942 CE LYS B 243 | 63.056 -17.681 | 70.242 | 1.00 54.69 |
| ATOM | 4943 NZ LYS B 243 | 62.456 -18.025 | 68.923 | 1.00 57.75 |
| MOTA MOTA | 4944 C LYS B 243 4945 O LYS B 243 | 61.793 -19.755 | 73.824 | 1.00 43.21 |
| ATOM | 4945 O LYS B 243 4946 N GLU B 244 | 61.432 -20.455 62.312 -20.257 | 72.884 | 1.00 42.92 |
| MOTA | 4947 CA GLU B 244 | 62.528 -21.687 | 74.935 75.085 | 1.00 45.77 1.00 47.72 |
| MOTA | 4948 CB GLU B 244 | 63.669 -21.925 | 76.075 | 1.00 50.89 |
| ATOM | 4949 CG GLU B 244 | 64.080 -23.378 | 76.208 | 1.00 57.16 |
| ATOM ATOM | 4950 CD GLU B 244 4951 CE1 GLU B 244 | 65.223 -23.564 | 77.173 | 1.00 57.74 |
| ATOM | 4952 OE2 GLU B 244 | 66.295 -22.967 65.049 -24.308 | 76.942 78.160 | 1.00 60.18 |
| ATOM | 4953 C GLU B 244 | 61.312 -22.507 | 75.505 | 1.00 61.59 1.00 47.78 |
| ATOM | 4954 O GLU B 244 | 61.376 -23.736 | 75.544 | 1.00 51.39 |
| ATOM | 4955 N VAL B 245 | 60.200 -21.851 | 75.805 | 1.00 43.31 |
| ATOM ATOM | 4956 CA VAL B 245 4957 CB VAL B 245 | 59.019 -22.589 | 76.230 | 1.00 43.55 |
| ATOM | 4958 CG1 VAL B 245 | 58.867 -22.514 57.665 -23.322 | 77.771 78.231 | 1.00 45.89 1.00 49.90 |
| ATOM | 4959 CG2 VAL B 245 | 60.131 -23.040 | 78.435 | 1.00 45.30 |
| MOTA | 4960 C VAL B 245 | 57.727 -22.115 | 75.565 | 1.00 41.01 |
| ATOM | 4961 C VAL B 245 | 56.659 -22.676 | 75.798 | 1.00 39.36 |
| ATOM | 4962 N PHE B 246 | 57.814 -21.101 | 74.716 | 1.00 34.37 |
| ATOM ATOM | 4963 CA PHE B 246 4964 CB PHE B 246 | 56.610 -20.602 55.986 -19.517 | 74.077 74.958 | 1.00 34.36 |
| ATOM | 4965 CG PHE B 246 | 54.542 -19.230 | 74.938 | 1.00 30.80 1.00 32.57 |
| ATOM | 4966 CD1 PHE B 246 | 53.548 -20.142 | 74.989 | 1.00 32.37 |
| ATOM | 4967 CD2 PHE B 246 | 54.174 -18.048 | 74.003 | 1.00 28.20 |
| ATOM | 4968 CE1 PHE B 246 | 52.207 -19.878 | 74.704 | 1.00 26.71 |
| ATOM ATOM | 4969 CE2 PHE B 246 4970 CL PHE B 246 | | 73.713 74.065 | 1.00 29.27 |
| MOTA | 4971 C PHE B 246 | | 74.005 72.682 | 1.00 26.18 1.00 35.32 |
| MOTA | 4972 O PHE B 246 | | 72.517 | 1.00 35.32 |
| MOTA | 4973 N GLU B 247 | | 71.683 | 1.00 37.00 |
| | | • | • | |

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| ATOM | | | 56.363 | -20.137 | 70.296 | 1.00 40.73 |
|--------------|---|---|------------------|--------------------|------------------|--------------------------|
| MOTA | | | 56.518 | 3 -21.347 | 69.370 | |
| ATOM | 4976 CG GLU B 247 | | 56.670 | -22.702 | 70.073 | |
| ATOM | 4977 CD GLU B 247 | | 55.381 | -23.214 | 70.718 | 1.00 55.29 |
| ATOM | 4978 OE1 GLU B 247 | | 54.887 | -22.601 | | |
| ATOM | 4979 OE2 GLU B 247 | | 54.859 | -24.246 | 70.241 | |
| ATOM | 4980 C GLU B 247 | | 55.090 | -19.379 | 69.939 | |
| ATOM | 4981 O GLU B 247 | | 54.129 | -19.960 | 69.436 | |
| ATOM | 4982 N PRO B 248 | | 55.076 | -18.064 | 70.182 | |
| ATOM | 4983 CD PRO B 248 4984 CA PRO B 248 | | 56.188 | -17.270 | 70.733 | |
| MOTA ATOM | | - | 53.935 | -17.188 | 69.916 | |
| MOTA | 4985 CB PRO B 248 4986 CG PRO B 248 | | 54.3/5 | -15.878 | 70.562 | |
| MOTA | 4987 C PRO B 248 | | 53.644 | -15.880 -16.990 | 70.233 | |
| ATOM | 4988 O PROB 248 | | 54 427 | -16.990 | | |
| ATOM | 4989 N GLU B 249 | | 52 262 | -10.808 | 67.604 | |
| ATOM | 4990 CA GLU B 249 | | 51 773 | -17.012 | 68.182 | |
| ATOM | 4991 CB GLU B 249 | | 50 374 | -17.366 | 66.828 66.645 | 1.00 29.35 |
| ATOM | 4992 CG GLU B 249 | | 50.284 | -18.867 | 66.787 | |
| ATOM | 4993 CD GLU B 249 | | 48.847 | -19.338 | 66.747 | 1.00 28.64 1.00 33.37 |
| ATOM | 4994 OE1 GLU B 249 | | 48.069 | -18.917 | 67.630 | 1.00 35.37 |
| ATOM | 4995 OE2 GLU B 249 | | 48.494 | -20.115 | 65.835 | 1.00 20.38 |
| ATOM | 4996 C GLU B 249 | | 51.700 | -15.273 | 66.650 | 1.00 28.25 |
| ATOM | 4997 O GLU B 249 | | 51.776 | -14.765 | 65.537 | 1.00 21.47 |
| ATOM | 4998 N VAL B 250 | | 51.561 | -14.564 | 67.768 | 1.00 21.77 |
| MOTA | 4999 CA VAL B 250 | | 51.459 | -13.110 | 67. 7 56 | 1.00 21.41 |
| ATOM | 5000 CB VAL B 250 | | 50.027 | -12.676 | 67.357 | 1.00 26.42 |
| MOTA | 5001 CG1 VAL B 250 | | | -13.196 | 68.378 | 1.00 20.96 |
| ATOM | 5002 CG2 VAL B 250 5003 C VAL B 250 | | | -11.166 | 67.243 | 1.00 24.68 |
| ATOM | | | | -12.608 | 69.168 | 1.00 22.88 |
| MOTA MOTA | 5004 O VAL B 250 5005 N TYR B 251 | | | -13.354 | 70.133 | 1.00 18.00 |
| MOTA | 5006 CA TYR B 251 | | | -11.359 | 69.295 | 1.00 20.28 |
| ATOM | 5007 CB TYR B 251 | | 52.40I | -10.823 -11.043 | 70.620 | 1.00 22.33 |
| ATOM | 5008 CG TYR B 251 | | 54.948 | -10.045 | 70.999 70.427 | 1.00 20.67 |
| ATOM | 5009 CD1 TYR B 251 | | 55.198 | -8.834 | 71.072 | 1.00 21.89 1.00 19.31 |
| ATOM | 5010 CE1 TYR B 251 | | 56.129 | -7.922 | 70.562 | 1.00 13.31 |
| ATOM | 5011 CD2 TYR B 251 | | | -10.321 | 69.254 | 1.00 18.72 |
| ATOM | 5012 CE2 TYR B 251 | | 56.580 | -9.417 | 68.734 | 1.00 22.71 |
| ATOM | 5013 CZ TYR B 251 | | 56.813 | -8.220 | 69.390 | 1.00 27.33 |
| ATOM | 5014 OH TYR B 251 | | 57.705 | -7.308 | 68.865 | 1.00 23.18 |
| MOTA | 5015 C TYR B 251 | | 52.134 | -9.349 | 70.732 | 1.00 25.71 |
| ATOM | 5016 O TYR B 251 | | 52.095 | -8.622 | 69.728 | 1.00 20.14 |
| MOTA | 5017 N LEU B 252 | | 51.834 | -8.930 | 71.958 | 1.00 21.13 |
| ATOM | 5018 CA LEU B 252 | | 51.533 | -7.532 | 72.252 | 1.00 24.61 |
| MOTA | 5019 CB LEU B 252 | | 50.154 | -7.373 | 72.897 | 1.00 22.88 |
| ATOM | 5020 CG LEU B 252 5021 CD1 LEU B 252 | | 48.915 | -7.435 | 1.996 | 1.00 23.73 |
| ATOM ATOM | 5022 CD2 LEU B 252 | | 48.779 47.697 | -8.792 | 71.360 | 1.00 23.18 |
| ATOM | 5023 C LEU B 252 | | 52.610 | -7.119 | 72.833 | 1.00 29.06 |
| ATOM | 5024 O LEU B 252 | | 53.064 | -7.044 -7.797 | 73.217 74.076 | 1.00 24.77 1.00 23.33 |
| MOTA | 5025 N LEU B 253 | | 53.011 | -5.786 | 73.071 | 1.00 23.33 |
| ATOM | 5026 CA LEU B 253 | | 54.057 | -5.209 | 73.911 | 1.00 20.14 |
| ATOM | 5027 CB LEU B 253 | | 55.304 | -4.946 | 73.051 | 1.00 25.33 |
| ATOM | 5028 CG LEU B 253 | | 56.490 | -4.210 | 73.688 | 1.00 18.34 |
| ATOM | 5029 CD1 LEU B 253 | | 57.062 | -5.044 | 74.829 | 1.00 14.11 |
| MOTA | 5030 CD2 LEU B 253 | | 57.552 | -3.953 | 72.624 | 1.00 19.60 |
| ATOM | 5031 C LEU B 253 | | 53.550 | -3.913 | 74.536 | 1.00 20.54 |
| ATOM | 5032 O. LEU B 253 | | 53.200 | -2.974 | 73.821 | 1.00 22.80 |
| MOTA | 5033 N. GLN B 254 | | 53.495 | -3.858 | 75.865 | 1.00 20.37 |
| MOTA | 5034 CA GLN B 254 | | 53.000 | -2.654 | 76.539 | 1.00 21.77 |
| ATOM | 5035 CB GLN B 254 | | 52.129 | -3.040 | 77.755 | 1.00 17.85 |
| ATOM | 5036 CG GLN B 254 | | | -2.815 | 79.124 | 1.00 32.51 |
| ATOM · | | | | -1.396 | 79.609 | 1.00 28.19 |
| ATCM | 5038 OE1 GLN B 254 | | | -0.996 | 80.124 | 1.00 26.96 |
| MOTA | 5039 NE2 GLN B 254 | | 53.603 | -0.619 | 79.432 | 1.00 16.80 |
| | | | | | | |

| MOTA | 5040 | С | GLN | B 254 | 9 | 54.211 | -1.793 | 76.887 | 1.00 20.15 |
|--------|-------------|-----|-------|-------|---|--------|--------|--------|--|
| | 5041 | 0 | | | | 55.186 | -2.254 | 77.497 | 1.00 20.11 |
| ATOM | | | | B 254 | | | | | |
| ATOM | 5042 | N | . LEU | в 255 | ! | 54.146 | -0.532 | 76.468 | 1.00 19.46 |
| ATOM | 5043 | CA | T.ETT | B 255 | | 55.268 | 0.386 | 76.614 | 1.00 15.99 |
| | | | | | | | | | • |
| ATOM | 5044 | CB | LEU | B 255 | | 55.692 | 0.831 | 75.211 | 1.00 18.15 |
| ATOM | 5045 | CG | LEU | в 255 | 9 | 56.143 | -0.316 | 74.296 | 1.00 21.80 |
| | | | | | - | 6.215 | 0.159 | 72.850 | 1.00 16.70 |
| MCTA . | 5046 | | | B 255 | | | | | |
| ATOM | 5047 | CD2 | LEU | B 255 | | 57.501 | -0.843 | 74.771 | 1.00 13.76 |
| ATOM | 5048 | С | LEH | B 255 | | 55.083 | 1.614 | 77.492 | 1.00 21.41 |
| - | | | | | | | | | |
| atom | 5049 | 0 | - LEU | B 255 | : | 55.379 | 2.741 | 77.065 | 1.00 18.40 |
| ATOM | 5050 | N | GLY | B 256 | 5 | 4.618 | 1.408 | 78.718 | 1.00 16.80 |
| | 5051 | CA | | B 256 | | 4.456 | 2.519 | 79.634 | 1.00 19.90 |
| ATOM | | | | | | | | | |
| ATOM. | 5052 | С | GLY | B 256 | | 55.816 | 3.181 | 79.818 | 1.00 17.68 |
| ATOM | 5053 | 0 | GLY | B 256 | - | 6.854 | 2.514 | 79.841 | 1.00 13.96 |
| | 5054 | N | | B 257 | | 55.824 | 4.497 | 79.936 | 1.00 19.55 |
| MOTA | | | | | | | | | |
| ATOM | 5055 | CA | THR | B 257 | | 57.081 | 5.205 | 80.098 | 1.00 19.47 |
| ATOM | 5056 | CB | THR | B 257 | | 7.044 | 6.547 | 79.340 | 1.00 21.49 |
| | | | | B 257 | | 5.989 | 7.365 | 79.858 | 1.00 17.43 |
| MOTA | 5057 | OG1 | | | | | | | |
| ATOM | 5058 | CG2 | THR | B 257 | 5 | 6.780 | 6.311 | 77.850 | 1.00 22.49 |
| ATOM | 5059 | С | THR | B 257 | = | 7.440 | 5.466 | 81.564 | 1.00 20.75 |
| | | | | | | 8.480 | 6.054 | 81.843 | 1.00 25.01 |
| MOTA | 5060 | 0 | | B 257 | | | | | |
| ATOM | 5061 | N | | B 258 | 5 | 6.618 | 5.004 | 82.504 | 1.00 17.23 |
| ATOM | 5062 | CA | ASP | B 258 | 5 | 6.929 | 5.277 | 83.906 | 1.00 17.42 |
| | | | | B 258 | | 5.744 | | 84.846 | 1.00 12.75 |
| ATOM | 5063 | CB | | | | | | | |
| MOTA | 5064 | CG | ASP | B 258 | 5 | 55.197 | 3.524 | 84.676 | 1.00 21.60 |
| ATOM | 5065 | С | ASP | B 258 | 5 | 8.245 | 4.718 | 84.460 | 1.00 16.09 |
| | 5066 | ō | | B 258 | | 8.667 | 5.116 | 85.542 | 1.00 22.07 |
| ATOM | | | | | | | | | |
| ATOM | 5067 | | | B 258 | = | 55.901 | 2.642 | 84.150 | 1.00 17.74 |
| ATOM | 5068 | OD2 | ASP | B 258 | 5 | 4.041 | 3.281 | 85.109 | 1.00 18.68 |
| | 5069 | N | | B 259 | | 8.879 | 3.746 | 83.779 | 1.00 20.98 |
| ATOM | | | | | | | | | |
| MOTA | 5070 | CD | PRO | B 259 | | 8.474 | 2.901 | 82.641 | 1.00 17.75 |
| ATOM | 5071 | CA | PRO | B 259 | 6 | 0.154 | 3.257 | 84.321 | 1.00 22.63 |
| ATOM | 5072 | CB | | в 259 | | 0.395 | 1.988 | 83.506 | 1.00 23.46 |
| | | | | | | | • | | |
| Mota | 5073 | CG | | B 259 | | 9.800 | 2:343 | 82.199 | 1.00 27.08 |
| MOTA | 5074 | С | PRO | B 259 | 6 | 1.305 | 4.284 | 84.172 | 1.00 23.86 |
| ATOM | 5075 | 0 | DRO | B 259 | 6 | 2.406 | 4.082 | 84.698 | 1.00 24.24 |
| | | | | | | | | | 1.00 20.49 |
| ATOM | 5076 | N | | B 260 | | 1.054 | 5.387 | 83.465 | |
| ATOM | 5077 | CA | LEU | в 260 | 6 | 2.080 | 6.417 | 83.262 | 1.00 15.17 |
| ATOM | 5078 | CB | UEU | B 260 | 6 | 1.626 | 7.408 | 82.185 | 1.00 17.03 |
| | | | | | | 1.431 | 6.881 | 80.760 | 1.00 16.02 |
| ATOM | 5079 | CG | | B 260 | | | | | |
| ATOM | 5080 | CD1 | LEU | в 260 | 6 | 0.703 | 7.915 | 79.901 | 1.00 17.03 |
| ATOM | 5081 | CD2 | LEU | B 260 | 6 | 2.803 | 6.546 | 80.163 | 1.00 18.58 |
| | 5082 | c | LEU | | | 2.449 | 7.194 | 84.541 | 1.00 22.45 |
| ATOM | | | | | | | | | |
| ATOM | 5083 | 0 | LEU | B 260 | 6 | 1.611 | 7.440 | 85.412 | 1.00 17.84 |
| ATOM | 5084 | N | LEU | B 261 | 6 | 3.713 | 7.588 | 84.635 | 1.00 22.90 |
| | 3085 | CA | | B 261 | | 4.219 | 8.332 | 85.782 | 1.00 26.34 |
| ATOM | - | | | | | | | | |
| ATOM | 5086 | CB | PEA | B 261 | 6 | 5.605 | 8.914 | 85.473 | 1.00 20.58 |
| ATOM | 3087 | CG | LEU | B 261 | 6 | 6.180 | 9.850 | 86.553 | 1.00 28.44 |
| | 5088 | | T.ETT | B 261 | 6 | 6.481 | 9.055 | 87.812 | 1.00 29.84 |
| ATOM | | | | | | | | | |
| ATOM | 5089 | | | B 261 | | 7.462 | 10.522 | 86.057 | 1.00 32.10 |
| ATOM | 5090 | С | LEU | B 261 | 6 | 3.315 | 9.475 | 86.227 | 1.00 27.61 |
| | 5091 | 0 | T.ETT | B 261 | 6 | 2.978 | 9.586 | 87.408 | 1.00 24.02 |
| ATOM | | | | | | | | | |
| ATOM | 5092 | Ŋ | GLU | B 262 | | 2.934 | 10.315 | 85.269 | 1.00 23.33 |
| MOTA | 5093 | CA | GLU | B 262 | 6 | 2.126 | 11.490 | 85.530 | 1.00 23.38 |
| | 5094 | CB | | B 262 | | 2.115 | 12.415 | 84.302 | 1.00 23.17 |
| MOTA | | | | | | | | | |
| ATOM | 5095 | CG | | B 262 | | 3.503 | 12.854 | 83.806 | 1.00 28.98 |
| ATOM | 5096 | CD | GLU | B 262 | 6 | 4.179 | 11.831 | 82.902 | 1.00 32.26 |
| | 5097 | CE1 | | B 262 | | 3.702 | 10.673 | 82.838 | 1.00 29.28 |
| ATOM | | | | | | | | | |
| ATOM | 5098 | OE2 | | B 262 | | 5.201 | 12.186 | 82.264 | 1.00 25.42 |
| ATOM | 5099 | С | GLU | B 262 | 6 | 0.693 | 11.249 | 85.976 | 1.00 23.25 |
| | 5100 | 0 | | B 262 | | 0.013 | 12.192 | 86.368 | 1.00 27.63 |
| ATOM | | | | | | | | 85.927 | The second secon |
| ATOM | 5101 | N | | B 263 | | 0.219 | 10.011 | _ | 1.00 22.25 |
| ATOM | 5102 | CA | ASP : | B 263 | 5 | 8.840 | 9.751 | 86.345 | 1.00 24.46 |
| | 5103 | CB | ASP | B 263 | | 8.214 | 8.659 | 85.465 | 1.00 20.94 |
| ATOM | | | | | | | | 85.659 | 1.00 25.30 |
| ATOM | 5104 | CG | ASP | B 263 | | 6.710 | 8.543 | | |
| ATOM | 5105 | OD1 | ASP : | B 263 | 5 | 5.995 | 8.318 | 84.656 | 1.00 21.82 |
| | | | | | | | | - | |

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| MOTA | 5106 | or | 2 ASP | В | 263 | 56. | 239 | 8. | 666 | 86. | 811 | 1.00 | 18.31 | ł |
|--------------|--------------|----------|------------|-----|------------|--------------|-----|------|------------|--------------|-----|------|----------------|---|
| MOTA | 5107 | 7 C | ASP | В | 263 | | 834 | | 339 | | 814 | | 26.39 | |
| MOTA | 5108 | 3 0 | ASP | В | 263 | | 437 | | 335 | | 179 | | 22.1 | |
| MOTA | 5109 | N G | TYR | В | 264 | | 155 | | 124 | | 648 | 1.00 | 25.8 | ī |
| ATOM | 5110 |) Cž | TYR | В | 264 | | 101 | | 864 | | 084 | | 30.96 | |
| MOTA | 5111 | CE | TYR | В | 264 | | 511 | | 055 | | 841 | 1.00 | 36.80 |) |
| MOTA | 5112 | CG | TYR | В | 264 | | 241 | 12. | 356 | | 645 | | 46.58 | |
| ATOM | 5113 | CI | 1 TYR | В | 264 | | 981 | | 166 | | 542 | | 47.03 | |
| ATOM | 5114 | CE | 1 TYR | В | 264 | | 654 | | 370 | | 364 | | 50.25 | |
| MOTA | 5115 | CE | 2 TYR | В | 264 | 59. | 197 | | 779 | | 565 | | 50.94 | |
| ATOM | 5116 | CE | 2 TYR | В | 264 | 59. | 876 | | 977 | | 396 | | 51.28 | |
| MOTA | 5117 | CZ | TYR | В | 264 | 59. | 600 | 14. | 769 | | 297 | | 52.21 | |
| ATOM | 5118 | OH | TYR | В | 264 | 60. | 268 | 15. | 961 | | 142 | | 49.65 | |
| ATOM | 5119 | C | TYR | В | 264 | 57. | 340 | 8. | 628 | 90. | 525 | | 31.04 | |
| MOTA | 5120 | 0 | TYR | В | 264 | 57. | | 8. | 181 | 91. | 657 | 1.00 | 24.50 |) |
| ATOM | 5121 | N | LEU | В | 265 | 56. | 491 | 8. | 074 | 89. | 666 | 1.00 | 26.68 | ļ |
| MOTA | 5122 | | | | 265 | 55. | | 6. | 900 | 90. | 086 | | 24.17 | |
| MOTA | 5123 | | | | | 54. | | 6. | 838 | 89. | 390 | 1.00 | 24.69 |) |
| ATOM | 5124 | | | | 265 | 53. | | 7. | 982 | | 761 | 1.00 | 26.00 |) |
| MOTA | 5125 | | 1 LEU | | 265 | 51. | | | 583 | 89. | | | 22.21 | |
| ATOM | 5126 | | 2 LEU | | 265 | 53. | | | 281 | | 238 | | 29.31 | |
| ATOM | 5127 | | LEU | | 265 | 56. | | | 568 | | 948 | | 25.83 | |
| MOTA | 5128 | 0 | LEU | | 265 | 55. | | | 512 | | 908 | | 21.74 | |
| MOTA | 5129 | N | SER | | 266 | 57. | | | 618 | 89. | | | 23.30 | |
| ATOM | 5130 | CA | SER | | 266 | 58. | | | 398 | 89. | | | 20.75 | |
| ATOM ATOM | 5131 5132 | CB OG | SER SER | | 266 266 | 58.3 59.3 | | | 900 | 88. | | | 19.67 | |
| ATOM | 5133 | C | SER | | 266 | 59. | | | 615 710 | 87. | | | 18.11 | |
| ATOM | 5134 | ō | SER | | 266 | 60.4 | | | 845 | 90. 90. | | | 23.01 17.74 | |
| ATOM | 5135 | N | LYS | | 267 | 60. | | | 707 | 91. | | | 24.25 | |
| ATOM | 5136 | CA | LYS | | | 61.9 | | | 916 | 91. | | | 23.79 | |
| ATOM | 5137 | CB | LYS | | | 62.0 | | | 153 | 92. | | | 23.71 | |
| MOTA | 5138 | CG | LYS | | | 60.9 | | | 582 | 93. | | | 27.29 | |
| ATOM | 5139 | CD | LYS | В | 267 | 61.0 | 059 | | 880 | 94. | | | 30.33 | |
| ATOM | 5140 | CE | LYS | | 267 | 60.0 | 067 | 5.5 | 535 | 95.3 | 273 | 1.00 | 30.90 | |
| MOTA | 5141 | NZ | LYS | | 267 | 60.1 | | 7.0 | 004 | 95. | | | 33.37 | |
| ATOM | 5142 | C | LYS | | 267 | 62.9 | | | 483 | 90. | | | 26.41 | |
| MOTA | 5143 | 0 | LYS | | 267 | 64.1 | | | 317 | 91. | | | 25.33 | |
| ATOM | 5144 | N | | | 268 | 62.5 | | | 288 | 89. | | | 22.18 | |
| MOTA | 5145 | CA | PHE | | 268 | 63.5 | | | 919 | 88. | | | 22.78 | |
| MOTA | 5146 | CB CG | PHE | | 268 | 62.8 | | | 171 | 87.3 | | | 20.55 | |
| MOTA MOTA | 5147 5148 | | PHE | | 268 268 | 62.3 | | -0.0 | 761 | 87.5 86.5 | | | 19.23 20.72 | |
| MOTA | 5149 | CD2 | | | 268 | 62.6 | | | 207 | 88. | | | 18.17 | |
| ATOM | 5150 | CE1 | | | | 61.3 | - | -1.3 | | 86.8 | | | 18.83 | |
| ATOM | 5151 | CE2 | | | 268 | 62.3 | | -1.1 | | 89.0 | | | 20.05 | |
| ATOM | 5152 | CZ | | | 268 | 61.6 | | -1.8 | | 88.3 | | 1.0' | 19.70 | |
| ATOM | 5153 | c | | | 268 | 64.1 | | 4.2 | | 87.7 | | 1.01 | 23.66 | |
| ATOM | 5154 | ō | PHE | | 268 | 63.4 | | 5.2 | | 87.6 | | 1.00 | 19.40 | |
| MOTA | 5155 | N | ASN I | | | 65.3 | | 4.2 | | 87.4 | | | 21.96 | |
| MOTA | 5156 | CA | ASN 1 | B 2 | 269 | 66.0 | | 5.3 | | 86.9 | | | 25.04 | |
| ATOM | 5157 | CB | ASN 1 | 3 2 | 269 | 67.2 | | 5.7 | | 87.8 | | | 25.68 | |
| MOTA | 5158 | CG | ASN I | 3 2 | 69 | 66.8 | 45 | 5.9 | 46 | 89.2 | 73 | 1.00 | 27.04 | |
| MOTA | 5159 | OD1 | ASN I | 3 2 | 69 | 65.8 | 32 | 6.5 | 57 | 89.5 | 79 | 1.00 | 28.81 | |
| ATOM | 5160 | ND2 | ASN I | | 69 | 67.6 | 59 | 5.4 | 19 | 90.1 | .76 | 1.00 | 31.12 | |
| ATOM | 5161 | С | ASN I | | | 66.5 | | 5.1 | .51 | 85.5 | | 1.00 | 25.87 | |
| ATOM | 5162 | 0 | ASN I | | 69 | 67.7 | | 5.3 | | 85.2 | | | 24.58 | |
| MOTA | 5163 | N | LEU E | | | 65.6 | | 4.7 | | 84.6 | | | 21.37 | |
| MOTA | 5164 | CA | LEU E | | 70 | 66.1 | | 4.4 | | 83.2 | | | 16.35 | |
| ATOM | 5165 | CB | LEU E | | 70 | 65.1 | | 3.4 | | 82.6 | | | 24.12 | |
| ATOM | 5166 | CG | LEU E | | 70 | 64.9 | | 2.1 | | 83.4 | | | 27.89 | |
| ATOM | 5167 | | LEU E | | 70 | 64.1 | | 1.1 | | 82.5 | | | 23.01 | |
| ATOM | 5168 | CD2 | LEU E | | 70 | 66.2 | | 1.5 | | 83.9 | | | 23.92 | |
| MOTA | 5169 | C | LEU E | | | 66.1 | | 5.6 | | 82.3 | | | 20.06 | |
| ATOM | 5170 | 0 N | LEU E | | | 65.6 | | 6.7 | | 82.6 81.1 | | 1.00 | 16.34 20.07 | |
| ATOM | 5171 | N . | SER E | 2 | 11 | 66.8 | 37 | 5.4 | <i>71</i> | | J J | 4.00 | 20.07 | |

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| | c177 | CA | SER B | 271 | | 66.989 | 6.546 | 80,200 | 1.00 21.20 |
|---------|--------|-----|--------|-----|---|--------|--------|--------|------------|
| MOTA | 5172 | | SER B | | | 68.437 | 6.621 | 79.714 | 1.00 21.80 |
| MOTA | 5173 | CB | | | | | 5.485 | 78.921 | 1.00 21.47 |
| MOTA | 5174 | OG | SER B | | | 68.772 | | 79.000 | 1.00 22.83 |
| ATOM | 5175 | С | SER B | | | 66.106 | 6.228 | | 1.00 16.12 |
| MOTA | 5176 | 0 | SER B | 271 | | 65.631 | 5.102 | 78.854 | 1.00 20.84 |
| MOTA | 5177 | N | ASN B | 272 | | 65.916 | 7.238 | 78.154 | |
| ATOM | 5178 | CA | ASN B | 272 | | 65.152 | 7.156 | 76.906 | 1.00 27.82 |
| ATOM | 5179 | CB | ASN B | 272 | | 65.263 | 8.478 | 76.123 | 1.00 30.30 |
| MOTA | 5180 | CG. | ASN B | 272 | | 64.198 | 9.456 | 76.475 | 1.00 37.83 |
| | 5181 | | ASN B | | | 64.167 | 10.575 | 75.946 | 1.00 37.72 |
| ATOM | 5182 | | | 272 | | 63.299 | 9.052 | 77.360 | 1.00 41.69 |
| MOTA | 5183 | C | ASN B | | | 65.701 | 6.088 | 75.974 | 1.00 26.88 |
| ATOM | | ō | ASN B | | | 64.967 | 5.280 | 75.412 | 1.00 23.12 |
| ATOM | 5184 | | VAL B | | | 67.012 | 6.160 | 75.774 | 1.00 20.40 |
| ATOM | 5185 | N | VAL B | | | 67.745 | 5.260 | 74.899 | 1.00 27.34 |
| ATOM | 5186 | CA | | | | 69.225 | 5.705 | 74.805 | 1.00 30.40 |
| MOTA | 5187 | CB | VAL B | 273 | | 70.036 | 4.691 | 74.029 | 1.00 34.98 |
| ATOM | 5188 . | | VAL B | | | | 7.057 | 74.115 | 1.00 33.57 |
| MOTA | 5189 | | VAL B | | • | 69.299 | 3.812 | 75.343 | 1.00 24.23 |
| MOTA | 5190 | С | VAL B | | • | 67.664 | 2.913 | 74.513 | 1.00 24.19 |
| ATOM | 5191 | 0 | VAL B | | | 67.590 | | 76.648 | 1.00 20.96 |
| ATOM | 5192. | N | ALA B | | | 67.690 | 3.580 | 77.151 | 1.00 20.30 |
| MOTA | 5193 | CA | ALA B | | | 67.589 | 2.220 | 78.646 | 1.00 19.09 |
| ATOM | 5194 | CB | ALA .B | | | 67.858 | 2.195 | | |
| ATOM | 5195 | С | ALA B | | | 66.172 | 1.729 | 76.863 | 1.00 18.23 |
| ATOM | 5196 | 0 | ALA B | 274 | | 65.962 | 0.567 | 76.525 | 1.00 20.77 |
| ATOM | 5197 | N | PHE B | 275 | | 65.207 | 2.631 | 77.003 | 1.00 18.50 |
| ATOM | 5198 | CA | PHE B | 275 | | 63.802 | 2.310 | 76.761 | 1.00 21.25 |
| ATOM | 5199 | CB | PHE B | | • | 62.941 | 3.546 | 77.037 | 1.00 22.24 |
| ATOM | 5200 | CG | PHE B | 275 | | 61.466 | 3.303 | 76.921 | 1.00 24.72 |
| ATOM | 5201 | CD1 | PHE B | 275 | | 60.815 | 2.483 | 77.826 | 1.00 23.64 |
| ATOM | 5202 | | PHE B | | | 60.732 | 3.893 | 75.907 | 1.00 27.31 |
| MOTA | 5203 | CEl | PHE B | 275 | | 59.450 | 2.254 | 77.722 | 1.00 27.82 |
| ATOM | 5204 | | PHE B | 275 | | 59.365 | 3.670 | 75.795 | 1.00 27.62 |
| ATOM | 5205 | CZ | PHE B | | | 58.727 | 2.851 | 76.701 | 1.00 25.78 |
| ATOM | 5206 | c | PHE .B | | | 63.642 | 1.860 | 75.305 | 1.00 24.47 |
| ATOM | 5207 | 0 | PHE B | | | 63.045 | 0.821 | 75.030 | 1.00 22.68 |
| ATOM | 5208 | N | LEU B | | | 64.183 | 2.648 | 74.378 | 1.00 23.85 |
| ATOM | 5209 | CA | LEU B | | | 64.128 | 2.330 | 72.946 | 1.00 21.28 |
| MOTA | 5210 | CB | LEU B | | | 64.814 | 3.421 | 72.134 | 1.00 19.87 |
| | 5211 | CG | | 276 | | 65.114 | 3.132 | 70.662 | 1.00 24.94 |
| MOTA | 5212 | | LEU B | | | 63.818 | 2.852 | 69.936 | 1.00 24.81 |
| MOTA | 5213 | CD2 | LEU B | 276 | | 65.840 | 4.312 | 70.018 | 1.00 21.01 |
| MOTA | 5214 | c | LEU B | 276 | | 64.841 | 1.021 | 72.653 | 1.00 22.33 |
| ATOM | 5215 | ŏ | LEU B | | | 64.348 | 0.191 | 71.886 | 1.00 20.73 |
| MOTA | 5216 | N | LYS B | | | 66.011 | 0.857 | 73.261 | 1.00 20.72 |
| MOTA | 5217 | CA | LYS 3 | | | 66.823 | -0.335 | 73.076 | 1.00 24.36 |
| ATOM | 5218 | CB | LYS B | | | 68.086 | -0.239 | 73.938 | 1.00 27.37 |
| ATOM | 5219 | CG | LYS 3 | 277 | | 69.303 | -0.973 | 73.381 | 1.00 35.58 |
| ATOM | 5220 | CD | LYS B | 277 | | 69.061 | -2.456 | 73.188 | 1.00 43.87 |
| ATOM | 5221 | CE | LYS B | | | 70.283 | -3.137 | 72.580 | 1.00 44.87 |
| ATOM | | | LYS B | | | 70.616 | -2.586 | 71.230 | 1.00 49.66 |
| ATOM | 5222 | NZ | LYS B | 277 | | 66.000 | -1.554 | 73.482 | 1.00 24.22 |
| MOTA | 5223 | C | LYS B | 277 | | 65.987 | -2.568 | 72.777 | 1.00 19.90 |
| ATOM | 5224 | 0 | | | | 65.319 | -1.454 | 74.624 | 1.00 22.32 |
| ATOM | 5225 | N | ALA B | 270 | | 64.476 | -2.544 | 75.114 | 1.00 21.71 |
| ATOM | 5226 | CA | ALA B | | | | -2.117 | 76.381 | 1.00 17.34 |
| ATOM | 5227 | CB | ALA B | 4/8 | | 63.752 | -2.896 | 74.031 | 1.00 22.68 |
| MOTA | 5228 | Ç | ALA B | 278 | | 63.459 | | 73.723 | 1.00 19.27 |
| MOTA | 5229 | 0 | ALA B | | | 63.231 | -4.068 | 73.464 | 1.00 24.79 |
| ATOM | 5230 | N | PHE B | | | 62.849 | -1.862 | 72.398 | 1.00 22.74 |
| ATOM | 5231 | CA | PHE B | | | 61.860 | -2.014 | 72.336 | 1.00 22.46 |
| ATOM | 5232 | CB | PHE B | | | 61.395 | -0.629 | 70.778 | 1.00 22.62 |
| ATOM | 5233 | CG | PHE B | | | 60.467 | -0.640 | | 1.00 22.02 |
| ATOM | 5234 | CD1 | PHE B | 279 | | 59.196 | -1.182 | 70.882 | 1.00 21.74 |
| MOTA | 5235 | CD2 | PHE B | 279 | | 60.862 | -0.078 | 69.567 | 1.00 27.02 |
| ATOM | 5236 | CEl | PHE B | 279 | | 58.325 | -1.162 | 69.799 | 1.00 27.02 |
| ATOM | 5237 | CE2 | PHE B | 279 | | 60.001 | -0.051 | 68.476 | 1.00 23.37 |
| 530 WAS | | | | | | | | | |

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| | 5536 | | | | 50 727 | 0 504 | 68.592 | 1.00 25.13 |
|--------------|--------------|---------|-------|-------|------------------|-------------------|------------------|------------|
| MOTA | 5238 | CZ | | в 279 | 58.727 | | | |
| ATOM | 5239 | C | PHE | B 279 | 62.472 | -2.768 | 71.212 | 1.00 23.60 |
| MOTA | 5240 | 0 | PHE | B 279 | 61.866 | -3.697 | 70.678 | 1.00 26.54 |
| | 5241 | N | | B 280 | 63.677 | -2.376 | 70.804 | 1.00 21.93 |
| MOTA | | | | | | | | |
| MOTA | 5242 | CA | | B 280 | 64.318 | | 69.680 | 1.00 23.70 |
| MOTA | 5243 | CB | ASN | B 280 | 65.520 | ~-2.248 | 69.164 | 1.00 22.63 |
| MOTA | 5244 | CG | ASN | B 280 | 65.107 | -0.937 | 68.505 | 1.00 30.83 |
| | | - | | | 64.094 | | 67.796 | 1.00 25.81 |
| MOTA | 5245 | OD1 | | B 280 | | | | |
| MOTA | 5246 | ND2 | ASN : | B-280 | 65.900 | 0.112 | 68.714 | 1.00 26.54 |
| MOTA | 5247 | С | ASN : | B 280 | 64.746 | -4.466 | 70.009 | 1.00 26.10 |
| | 5248 | 0 | | B 280 | - 64.775 | -5.321 | 69.124 | 1.00 26.16 |
| MOTA | | | | | 65.080 | | 71.272 | 1.00 26.10 |
| MOTA | 5249 | N | ILE : | | | | | |
| MOTA | 5250 | CA | ILE : | B 291 | 65.485 | | 71.667 | 1.00 25.81 |
| MOTA | 5251 | CB | ILE : | B 281 | 66.006 | -6.098 | 73.124 | 1.00 28.50 |
| ATOM | 5252 | CG2 | | | 66.046 | -7.527 | 73.648 | 1.00 28.53 |
| | | | | | | -5.454 | 73.173 | , |
| MOTA | 5253 | CG1 | | B 281 | 67.392 | | | |
| MOTA | 5254 | CD1 | ILE 1 | B 281 | 68.038 | | 74.541 | |
| ATOM | 5255 | С | ILE I | 3 281 | 64.320 | -7.030 | 71.507 | 1.00 25.77 |
| | 5256 | 0 | | 3 281 | 64.484 | -8.131 | 70.982 | 1.00 23.39 |
| ATOM | | | | | | -6.618 | | 1.00 21.30 |
| MOTA | 5257 | N | VAL | | 63.139 | | | |
| ATOM | 5258 | CA | VAL I | | 61.961 | -7.465 | 71.813 | 1.00 22.90 |
| ATOM | 5259 | CB | VAL I | 3 282 | 60.703 | -6 <i>.</i> 775 | 72.387 | 1.00 24.07 |
| ATOM | 5260 | | VAL I | | 59.464 | -7.611 | 72.093 | 1.00 22.28 |
| | | | VAL | | 60.865 | -6.587 | 73.906 | 1.00 26.89 |
| ATOM | 5261 | | | | | | | |
| ATOM | 5262 | С | VAL I | | 61.718 | -7,795 | 70.339 | 1.00 23.87 |
| ATOM | 5263 | 0 | VAL I | 3 282 | 61.462 | -8.949 | 69.978 | 1.00 22.65 |
| ATOM | 5264 | N | ARG I | 3 293 | 61.799 | -6.779 | 69.488 | 1.00 23.19 |
| | | CA | ARG I | | 61.576 | -6.971 | 68.060 | 1.00 27.95 |
| ATOM | 5265 | | | | | | 67.359 | 1.00 25.48 |
| ATOM | 5266 | CB | ARG I | | 61.510 | -5.612 | | |
| ATOM | 5267 | CG | ARG I | 3 283 | 60.337 | -4.760 | 67.838 | 1.00 26.55 |
| ATOM | 5268 | CD | ARG I | 283 | 60.442 | -3.333 | 67.339 | 1.00 31.52 |
| | 5269 | NE | ARG I | | 60.210 | -3.208 | 65.908 | 1.00 24.43 |
| ATOM | | | | | | -2.414 | 65.116 | 1.00 26.45 |
| MOTA | 5270 | CZ | ARG I | | 60.915 | | | |
| MOTA | 5271 | NH1 | ARG I | 3 283 | 61.902 | -1.676 | 65.622 | 1.00 26.04 |
| ATOM | 5272 | NH2 | ARG F | 283 | 60.634 | ~2.356 | 63.825 | 1.00 29.64 |
| ATOM | 5273 | С | ARG I | | 62.634 | -7.855 | 67.402 | 1.00 32.04 |
| | | | ARG I | | 62.341 | -8.552 | 66.431 | 1.00 29.76 |
| MOTA | 5274 | 0 | | | | | | |
| MOTA | 5275 | N | GLU E | | 63.859 | -7.821 | 67.923 | 1.00 31.50 |
| MOTA | 5276 | CA | GLU F | 3 284 | 64.934 | -8.646 | 67.381 | 1.00 32.42 |
| ATOM | 5277 | CB | GLU F | 284 | 66.289 | -8.260 | 67.992 | 1.00 38.31 |
| | | CG | GLU E | | 66.798 | -6.864 | 67.640 | 1.00 48.93 |
| ATOM | 5278 | | | | | | 68.362 | 1.00 56.28 |
| MOTA | 5279 | CD | GLU E | | 68.102 | -6.518 | | |
| MOTA | 5280 | OE1 | GLU E | 284 | 69.084 | -7.281 | 68.222 | 1.00 57.37 |
| ATOM | 5281 | OE2 | GLU E | 284 | 68.150 | -5.485 | 69.069 | 1.00 55.42 |
| MOTA | 5282 | С | GLU E | | 64.638 | -10.105 | 67.714 | 1.00 31.93 |
| | | | | | 64.899 | -11.001 | 66.913 | 1.00 28.26 |
| ATOM | 5283 | 0 | GLU E | | | | | |
| ATOM | 5284 | N | VAL E | | 64.089 | -10.340 | 68.901 | 1.00 28.09 |
| MOTA | 5285 | CA | VAL E | 285 | 63.765 | -11.697 | 69.325 | 1.00 30.67 |
| ATOM | 5286 | CB | VAL E | 285 | 63.687 | -11.802 | 70.863 | 1.00 28.33 |
| | | | VAL E | | | -13.206 | 71.262 | 1.00 29.84 |
| ATOM | 5287 | | | | | | | 1.00 26.93 |
| MOTA | 5288 | CG2 | VAL E | | | -11.470 | 71.478 | |
| ATOM | 5289 | С | VAL E | 285 | 62.460 | -12.265 | 68.758 | 1.00 31.19 |
| | 5290 | ō | VAL E | 285 | 62.422 | -13.423 | 68.349 | 1.00 31.38 |
| ATOM | | | PHE B | 295 | | -11.460 | 68.729 | 1.00 28.21 |
| ATOM | 5291 | N | | | | | | |
| MOTA | 5292 | CA | PHE B | | | -11.948 | 68.249 | 1.00 25.71 |
| MOTA | 5293 | CB. | PHE B | 286 | 59.064 | -11.853 | 69.374 | 1.00-24.57 |
| ATOM | 5294 | CG | PHE B | 286 | 59.311 | ~12.804 | 70.514 | 1.00 26.87 |
| | | CD1 | PHE B | 286 | | -12.331 | 71.779 | 1.00 25.16 |
| ATOM | 5295 | CDI | FAD D | 200 | | -14.180 | 70.319 | 1.00 22.51 |
| ATOM | 5296 | | PHE B | -36 | | | | |
| ATOM: | 5297 | CE1 | PHE B | 286 | | -13.213 | 72.833 | 1.00 22.92 |
| ATOM | 5298 | CE2 | PHE B | 236 | 59.433 | -15.063 | 71.362 | 1.00 21.99 |
| | | cz | PHE B | 286 | | -14.578 | 72.626 | 1.00 26.75 |
| ATOM | 5299 | | PHE B | 206 | | -11.318 | 66.993 | 1.00 25.90 |
| ATOM | 5300 | C | PHE B | 200 | | | | 1.00 22.84 |
| ATOM: | 5301 | 0 | PHE B | 286 | | -11.630 | 66.620 | |
| | | | | | | 46 454 | | |
| ZUVW. | | N | GLY B | 287 | 60.272 | -10.451 | 66.329 | 1.00 28.27 |
| MOTA MOTA | 5302 5303 | N CA | GLY B | 287 | 60.272 59.756 | -10.451 -9.814 | 66.329 65.130 | 1.00 28.27 |

| ATOM | 5304 | С | GLY B 287 | | 58.765 | -8.719 | 65.498 | 1.00 29.17 |
|--------|------|-----|-------------|---|---------|--------|--------|------------|
| | | | | | | | | |
| ATCM | 5305 | | GLY B 287 | | 58.786 | -8.216 | 56.517 | 1.00 22.88 |
| ATOM | 5306 | N | GLU B 288 | | 57.896 | -8.361 | 64.558 | 1.00 26.77 |
| ATOM | 5307 | CA | GLU B 288 | | 56.893 | -7.324 | 64.754 | 1.00 25.38 |
| ATOM | 5308 | CB | GLU B 288 | | 56.405 | -6.791 | 63.405 | 1.00 29.51 |
| ATCM- | 5309 | CG | GLU B 288 | | 57.430 | -6.003 | 62.605 | 1.00 36.06 |
| | | CD | | | | | | |
| MOTA | 5310 | | | | 57.906 | -4.769 | 63.347 | 1.00 41.10 |
| ATCM | 5311 | | 1 GLU B 288 | | 57.058 | -4.055 | 63.919 | 1.00 41.19 |
| MOTA | 5312 | OE: | 2 GLU B 288 | | 59.125 | -4.503 | 63.348 | 1.00 44.69 |
| ATOM | 5313 | С | -GLU B 288 | | 55.682 | -7.819 | 65.527 | 1.00 27.87 |
| MOTA | 5314 | 0 | GLU B 288 | | .55.209 | -8.931 | 65.308 | 1.00 26.80 |
| | 5315 | N | GLY B 289 | | 55.176 | ~6.973 | 66.419 | 1.00 24.53 |
| MOTA | | | | | | -7.326 | - | |
| ATOM | 5316 | CA | GLY B 289 | | 54.006 | | 67.204 | 1.00 29.17 |
| ATOM | 5317 | С | GLY B 289 | | 53.015 | -6.171 | 67.244 | 1.00 30.46 |
| ATOM | 5318 | 0 | GLY B 289 | | 53.005 | -5.326 | 66.358 | 1.00 26.17 |
| ATOM | 5319 | N | VAL B 290 | | 52.171 | -6.142 | 68.268 | 1.00 23.95 |
| ATOM | 5320 | CA | VAL B 290 | | 51.194 | -5.079 | 68.440 | 1.00 22.25 |
| ATOM | 5321 | CB | VAL B 290 | | 49.794 | -5.655 | 68.783 | 1.00 18.71 |
| ATOM | 5322 | CGI | | • | 48.810 | -4.525 | 69.047 | 1.00 22.67 |
| | 5323 | CG2 | | | 49.289 | -6.504 | 67.629 | 1.00 19.26 |
| ATOM | | | | | | | | |
| ATOM | 5324 | C | VAL B 290 | | 51.722 | -4.232 | 69.593 | 1.00 21.55 |
| ATOM | 5325 | 0 | VAL B 290 | | 51.960 | -4.741 | 70.687 | 1.00 21.32 |
| MOTA | 5326 | N | TYR B 291 | | 51.913 | -2.941 | 69.346 | 1.00 21.06 |
| MOTA | 5327 | CA | TYR B 291 | | 52.479 | -2.063 | 70.357 | 1.00 19.29 |
| ATOM | 5328 | CB | TYR B 291 | | 53.582 | -1.216 | 69.711 | 1.00 20.40 |
| ATOM | 5329 | CG | TYR B 291 | | 54.553 | -2.072 | 68.918 | 1.00 23.09 |
| ATOM | 5330 | CD1 | | | 54.740 | -1.875 | 67.549 | 1.00 19.52 |
| | 5331 | CE1 | | | 55.580 | -2.712 | 66.809 | 1.00 20.67 |
| ATOM | | | | | | | 69.527 | |
| ATOM | 5332 | CD2 | | | 55.234 | -3.122 | | 1.00 22.88 |
| MOTA | 5333 | CE2 | | | 56.070 | -3.960 | 68.800 | 1.00 26.04 |
| ATOM · | 5334 | CZ | TYR B 291 | | 56.235 | -3.752 | 67.442 | 1.00 23.44 |
| ATOM | 5335 | OH | TYR B 291 | | 57.027 | -4.612 | 66.722 | 1.00 28.02 |
| MOTA | 5336 | С | TYR B 291 | | 51.465 | -1.180 | 71.068 | 1.00 26.89 |
| ATOM | 5337 | 0 | TYR B 291 | | 50.668 | -0.479 | 70.429 | 1.00 20.26 |
| ATOM | 5338 | N | LEU B 292 | | 51.522 | -1.204 | 72.399 | 1.00 21.75 |
| | 5339 | CA | LEU B 292 | | 50.604 | -0.426 | 73.227 | 1.00 22.11 |
| MOTA | | | | | 49.765 | -1.369 | | 1.00 20.92 |
| ATOM | 5340 | CB | LEU B 292 | | | | 74.088 | |
| ATOM | 5341 | CG | LEU B 292 | | 49.091 | -2.542 | 73.375 | 1.00 22.94 |
| ATOM | 5342 | CD1 | | | 48.328 | -3.362 | 74.411 | 1.00 21.03 |
| ATOM | 5343 | CD2 | LEU B 292 | | 48.149 | -2.043 | 72.281 | 1.00 18.04 |
| ATOM | 5344 | C | LEU B 292 | | 51.330 | 0.557 | 74.147 | 1.00 21.59 |
| ATOM | 5345 | 0 | LEU B 292 | | 52.514 | 0.404 | 74.426 | 1.00 19.96 |
| ATOM | 5346 | N | GLY B 293 | | 50.606 | 1.571 | 74.613 | 1.00 23.31 |
| ATOM | 5347 | CA | GLY B 293 | | 51.195 | 2.537 | 75.521 | 1.00 20.76 |
| | 5348 | C | GLY B 293 | | 51.163 | 1.979 | 76.930 | 1.00 26.15 |
| ATOM | | | | | 51.263 | | 77.133 | 1.00 20.96 |
| MCTA | 5349 | 0 | | | | 0.765 | | |
| ATOM | 5350 | N | GLY B 294 | | 51.017 | 2.859 | 77.914 | 1.00 24.63 |
| ATOM | 5351 | CA | GLY B 294 | | 50.980 | 2.407 | 79.293 | 1.00 20.00 |
| ATOM | 5352 | С | GLY B 294 | | 51.176 | 3.538 | 80.285 | 1.00 22.59 |
| ATOM | 5353 | 0 | GLY B 294 | | 51.145 | 4.719 | 79.916 | 1.00 17.46 |
| ATCM | 5354 | N | GLY B 295 | | 51.373 | 3.179 | 81.551 | 1.00 17.10 |
| ATOM | 5355 | CA | GLY B 295 | | 51.577 | 4.180 | 82.582 | 1.00 16.52 |
| | 5356 | c | GLY B 295 | | 52.695 | 5.145 | 82.232 | 1.00 19.54 |
| ATOM | | | | | | | 81.732 | 1.00 16.31 |
| ATOM | 5357 | 0 | GLY B 295 | | 53.738 | 4.737 | | |
| ATOM | 5358 | N | GLY B 296 | | 52.467 | 6.430 | 82.497 | 1.00 21.93 |
| ATCM | 5359 | CA | GLY B 296 | | 53.448 | 7.465 | 82.207 | 1.00 20.05 |
| ATOM | 5360 | С | GLY B 296 | | 52.869 | 8.750 | 82.759 | 1.00 22.20 |
| ATOM | 5361 | 0 | GLY B 296 | | 51.790 | 9.160 | 82.336 | 1.00 20.48 |
| ATOM | 5362 | N | TYR B 297 | | 53.573 | 9.402 | 83.682 | 1.00 20.93 |
| ATOM | 5363 | CA | TYR B 297 | | 53.025 | 10.598 | 84.306 | 1.00 23.25 |
| | 5364 | CB | TYR B 297 | | 52.731 | 10.284 | 85.774 | 1.00 19.93 |
| ATOM | | | TIN 2 227 | | | | | 1.00 24.76 |
| ATOM | 5365 | CG | TYR B 297 | | 52.041 | 8.944 | 85.900 | 1 00 21 07 |
| ATOM | 5366 | CD1 | TYR B 297 | | 52.779 | 7.758 | 85.936 | 1.00 21.97 |
| ATOM | 5367 | CE1 | TYR B 297 | | 52.148 | 6.514 | 85.912 | 1.00 19.79 |
| ATCM | 5368 | CD2 | TYR B 297 | | 50.653 | 8.850 | 85.849 | 1.00 20.86 |
| ATOM | 5369 | CE2 | TYR B 297 | | 50.012 | 7.612 | 85.822 | 1.00 19.57 |

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| ATOM | 1 5370 | CZ TYR B 297 | 50.75 | 8 6.457 | 85.851 | 1 00 22 00 |
|--------|--|---------------|--------|----------|-----------|------------|
| ATOM | 5371 | OH TYR B 297 | 50.10 | | | |
| ATOM | 5372 | C TYR B 297 | 53.83 | | | |
| ATOM | | O TYR B 297 | 53.45 | | | |
| ATOM | | N HIS B 298 | 54.97 | | | , |
| ATOM | _ | | | | | |
| ATOM | | | 55.78 | | · - · - • | |
| | | CB HIS B 298 | 57.27 | | 83.534 | 1.00 22.88 |
| ATOM | | CG HIS B 298 | 58.09 | | 83.502 | 1.00 25.13 |
| ATOM | 5378 | CD2 HIS B 298 | 58.40 | 6 14.791 | 82.482 | |
| ATOM | 5379 1 | ND1 HIS B 298 | 58.61 | 7 14.536 | 84.641 | |
| MOTA | | CE1 HIS B 298 | 59.20 | 9 15.674 | 84.323 | |
| ATOM | 5381 1 | WE2 HIS B 298 | 59.09 | | 83.019 | |
| ATOM | 5382 (| HIS B 298 | 55.589 | | 81.795 | |
| MOTA | 5383 C | HIS B 298 | 56.08 | | 80.923 | |
| MOTA | 5384 N | PRO B 299 | 54.90 | | 81.496 | |
| MOTA | 5385 0 | D PRO B 299 | 54.388 | | 82.447 | |
| ATOM | 5386 C | A PRO B 299 | 54.616 | | 80.127 | |
| ATOM | | B PRO B 299 | 53.952 | | | |
| ATOM | | G PRO B 299 | 54.583 | | 80.342 | 1.00 27.76 |
| ATOM | 5389 C | | | | 81.656 | 1.00 27.97 |
| ATOM | 5390 O | | 55.815 | | | 1.00 27.08 |
| ATOM | 5391 N | | 55.738 | | 78.057 | 1.00 28.58 |
| MOTA | | | 56.925 | | 79.668 | 1.00 27.30 |
| ATOM | | | 58.114 | | 78.824 | 1.00 27.17 |
| ATOM | | | 59.173 | | 79.466 | 1.00 31.65 |
| | | | 58.684 | | 79.921 | 1.00 31.61 |
| MOTA | | D1 TYR B 300 | 57.414 | | 79.582 | 1.00 32.71 |
| ATOM | | E1 TYR B 300 | 56.971 | 19.568 | 80.014 | 1.00 38.52 |
| ATOM | and the second s | D2 TYR B 300 | 59.499 | 18.670 | 80.701 | 1.00 30.92 |
| MOTA | | E2 TYR B 300 | 59.072 | 19.517 | 81.138 | 1.00 32.13 |
| ATOM | 5399 C | | 57.808 | 20.361 | 80.795 | 1.00 39.17 |
| ATOM | 5400 OF | | 57.374 | 21.585 | 81.252 | 1.00 43,90 |
| MOTA | 5401 C | TYR B 300 | 58.731 | 14.218 | 78.572 | 1.00 25.20 |
| ATOM | 5402 O | TYR B 300 | 59.106 | 13.894 | 77.445 | 1.00 25.15 |
| ATOM | 5403 N | ALA B 301 | 58.845 | 13.419 | 79.628 | 1.00 20.55 |
| MOTA | , 5404 CA | | 59.414 | 12.080 | 79.508 | 1.00 22.12 |
| ATOM | 5405 CE | B ALA B 301 | 59.417 | 11.388 | 80.874 | 1.00 17.09 |
| ATOM | 5406 C | ALA B 301 | 58.608 | 11.260 | 78.505 | 1.00 15.20 |
| MOTA | 5407 O | ALA B 301 | 59.161 | 10.629 | 77.613 | 1.00 17.12 |
| ATOM | 5408 N | LEU B 302 | 57.295 | 11.290 | 78.667 | 1.00 18.02 |
| MOTA | 5409 CA | LEU B 302 | 56.381 | 10.553 | 77.815 | 1.00 19.88 |
| MOTA | 5410 CB | LEU B 302 | 54.957 | 10.702 | 78.362 | 1.00 21.72 |
| ATOM · | 5411 CG | LEU B 302 | 53.767 | 10.118 | 77.606 | 1.00 31.08 |
| ATOM | 5412 CD | 1 LEU B 302 | 52.576 | 9.980 | 78.549 | 1.00 31.35 |
| ATOM | 5413 CD | 2 LEU B 302 | 53.434 | 11.011 | 76.415 | 1.00 31.33 |
| ATOM | 5414 C | LEU B 302 | 56.445 | 10.988 | 76.351 | 1.00 27.11 |
| ATOM : | 5415 O | LEU B 302 | 56.473 | 10.149 | 75.449 | 1.00 21.13 |
| ATOM | 5416 N | | 56.472 | 12.293 | 76.115 | 1.00 21.76 |
| ATOM | 5417 CA | ALA B 303 | 56.516 | 12.811 | 74.755 | 1.00 17.69 |
| ATOM | 5418 CB | ALA B 303 | 56.357 | 14.326 | 74.780 | 1.00 17.79 |
| ATOM | 5419 C | ALA B 303 | 57.803 | 12.425 | | 1.00 24.50 |
| ATOM | 5420 O | ALA B 303 | 57.781 | | 74.040 | 1.00 20.84 |
| MOTA | 5421 N | ARG B 304 | 58.930 | 11.968 | 72.891 | 1,00 19.33 |
| MOTA | 5422 CA | ARG B 304 | | | 74.723 | 1.00 21.08 |
| MOTA | 5423 CB | | 60.215 | 12.269 | 74.120 | 1.00 25.56 |
| | 5424 CG | ARG B 304 | 61.375 | | 74.962 | 1.00 18.37 |
| MOTA | | ARG B 304 | 61.427 | 14.356 | 75.072 | 1.00 23.12 |
| MOTA | 5425 CD | ARG B 304 | 62.797 | | 75.624 | 1.00 29.00 |
| MOTA | 5426 NE | ARG B 304 | 63.073 | | 76.789 | 1.00 33.28 |
| MOTA | 5427 CZ | ARG B 304 | 64.271 | 13.689 | 77.283 | 1.00 30.24 |
| MOTA | 5428 NH1 | | 65.363 | 14.194 | 76.723 | 1.00 24.98 |
| TOM | | ARG B 304 | 64.365 | 12.896 | 78.333 | 1.00 36.15 |
| MOT | 5430 C | ARG B 304 | 60.406 | | | 1.00 20.46 |
| LTCM | 5431 0 | ARG B 304 | 60.850 | | | 1.00 18.70 |
| MOT | 5432 N | ALA B 305 | 60.070 | | | 1.00 22.48 |
| TOM . | 5433 CA | ALA B 305 | 60.226 | | | 1.00 19.70 |
| MOT | 5434 CB | ALA B 305 | 59.847 | | | 1.00 24.24 |
| TOM | 5435 C | ALA B 305 | 59.407 | 7.930 | | 1.00 15.82 |
| | | | | • • | | |

| ATOM | 5436 | 0 ALA B 305 | 59.938 | 7.184 | 72.888 | 1.00 19.12 |
|--------------|-----------------------|--------------------------------|------------------|-----------------|------------------|--------------------------|
| MOTA | 5437 | - | 58.113 | 8.230 | 73.659 | 1.00 18.65 |
| MOTA | 5438 | | 57.298 | 7.668 | 72.600 | 1.00 19.57 |
| MOTA MOTA | 5439 5440 | | 55.800 55.301 | 7.856 | 72.893 | 1.00 18.26 |
| ATOM | 5441 | | 54.087 | 6.911 7.025 | 73.953 74.708 | 1.00 20.71 1.00 23.94 |
| MOTA | 5442 | | 53.988 | 5.870 | 75.513 | 1.00 24.73 |
| ATOM | 5443 | CE3 TRP B 306 | 53.073 | 7.991 | 74.780 | 1.00 26.01 |
| ATOM | 5444 | | 55.872 | 5.721 | 74.326 | 1.00 20.04 |
| ATOM | 5445 | | 55.092 | 5.093 | 75.260 | 1.00 19.17 |
| ATOM ATOM | 5446 5447 | CZ2 TRP B 306 CZ3 TRP B 306 | 52.912 52.001 | 5.655 7.779 | 76.385 75.646 | 1.00 28.04 |
| ATOM | 5448 | CH2 TRP B 306 | 51.930 | 6.619 | 76.437 | 1.00 28.68 1.00 31.22 |
| ATOM | 5449 | C TRP B 306 | 57.665 | 8.223 | 71.226 | 1.00 23.48 |
| MOTA | 5450 | O TRP B 306 | 57.416 | 7.574 | 70.212 | 1.00 22.38 |
| MOTA | 5451 | N THR B 307 | 58.262 | 9.412 | 71.176 | 1.00 22.36 |
| ATOM ATOM | 5452 5453 | CA THR B 307 CB THR B 307 | 58.672 59.143 | 9.953 11.417 | 69.880 69.986 | 1.00 25.94 1.00 25.88 |
| ATOM | 5454 | OG1 THR B 307 | 58.015 | 12.261 | 70.258 | 1.00 25.88 |
| ATOM | 5455 | CG2 THR B 307 | 59.827 | 11.864 | 68.686 | 1.00 22.52 |
| ATOM | 5456 | C THR B 307 | 59.815 | 9.078 | 69.350 | 1.00 30.09 |
| MOTA | 5457 | O THR B 307 | 59.922 | 8.834 | 68.144 | 1.00 25.82 |
| ATOM ATOM | 5458 5459 | N LEU B 308 CA LEU B 308 | 60.664 61.773 | 8.596 7.734 | 70.258 69.857 | 1.00 27.54 |
| ATOM | 5460 | CB LEU B 308 | 62.691 | 7.424 | 71.054 | 1.00 26.76 1.00 24.24 |
| MOTA | 5461 | CG LEU B 308 | 63.420 | 8.614 | 71.718 | 1.00 31.16 |
| MOTA | 5462 | CD1 LEU B 308 | 64.282 | 8.147 | 72.877 | 1.00 24.71 |
| MOTA | 5463 | CD2 LEU B 308 | 64.289 | 9.325 | 70.700 | 1.00 24.59 |
| MOTA MOTA | 5464 5465 | C LEU B 308 O LEU B 308 | 61.184 61.609 | 6.443 5.961 | 69.287 68.234 | 1.00 27.20 1.00 23.52 |
| ATOM | 5466 | N ILE B 309 | 60.190 | 5.898 | 69.980 | 1.00 25.32 |
| MOTA | 5467 | CA ILE B 309 | 59.537 | 4.679 | 69.530 | 1.00 25.14 |
| MOTA | 5468 | CB ILE B 309 | 58.387 | 4.266 | 70.485 | 1.00 27.05 |
| MOTA | 5469 5470 | CG2 ILE B 309 CG1 ILE B 309 | 57.646 | 3.058 | 69.926 | 1.00 23.57 |
| ATOM ATOM | 5471 | CD1 ILE B 309 | 58.952 59.927 | 3.947 2.793 | 71.868 71.868 | 1.00 22.98 1.00 24.25 |
| ATOM | 5472 | C ILE B 309 | 58.958 | 4.885 | 68.133 | 1.00 25.41 |
| MOTA | 5473 | O ILE B 309 | 59.177 | 4.064 | 67.243 | 1.00 22.13 |
| MOTA | 5474 | N TRP B 310 | 58.232 | 5.984 | 67.943 | 1.00 27.45 |
| ATOM ATOM | 5475 5476 | CA TRP B 310 CB TRP B 310 | 57.618 56.721 | 6.266 7.505 | 66.648 66.715 | 1.00 29.27 1.00 27.00 |
| ATOM | 5477 | CG TRP B 310 | 56.112 | 7.847 | 65.378 | 1.00 27.00 |
| ATOM | 5478 | CD2 TRP B 310 | 55.172 | 7.061 | 64.633 | 1.00 27.50 |
| ATOM | 5479 | CE2 TRP B 310 | 54.947 | 7.729 | 63.408 | 1.00 30.47 |
| MOTA MOTA | 5480 5481 | CE3 TRP B 310 CD1 TRP B 310 | 54.500 56.406 | 5.856 | 64.877 | 1.00 29.85 |
| ATOM | 5482 | NE1 TRP B 310 | 55.713 | ዖ.929 ⋅.865 | 64.597 63.415 | 1.00 29.76 1.00 26.71 |
| MOTA | 5483 | CZ2 TRP B 310 | 54.076 | 234 | 62.429 | 1.00 28.23 |
| ATOM | 5484 | CZ3 TRP B 310 | 53.636 | 5.362 | 63.901 | 1.00 30.24 |
| ATOM | 5485 | CH2 TRP B 310 | 53.433 | 6.053 | 62.692 | 1.00 27.63 |
| ATOM ATOM | 5486 5487 | C TRP B 310 O TRP B 310 | 58.629 58.378 | 6.424 | 65.520 | 1.00 30.16 |
| ATOM | 5488 | N CYS B 311 | 59.762 | 5.964 7.069 | 64.410 65.793 | 1.00 30.04 1.00 24.26 |
| ATOM | 5489 | CA CYS B 311 | 60.782 | 7.233 | 64.764 | 1.00 27.97 |
| MOTA | 5490 | CB CYS B 311 | 61.893 | 8.157 | 65.252 | 1.00 28.21 |
| ATOM | 5491 | SG CYS B 311 | 61.422 | 9.905 | 65.381 | 1.00 33.38 |
| MOTA | 5492 | C CYS B 311 O CYS B 311 | 61.380 | 5.886 | 64.351 63.172 | 1.00 30.02 |
| MOTA MOTA | 5493 5494 | O CYS B 311 N GLU B 312 | 61.670 61.570 | 5.660 5.001 | 65.327 | 1.00 25.45 1.00 31.59 |
| ATOM | 5495 | CA GLU B 31∠ | 62.111 | 3.669 | 65.067 | 1.00 33.48 |
| MOTA | 5496 | CE GLU B 312 | 62.142 | 2.843 | 66.352 | 1.00 34.78 |
| MOTA | 5497 | CG GLU B 312 | 63.487 | 2.307 | 66.758 | 1.00 39.45 |
| MOTA | 5498 | CD GLU B 312 OE1 GLU B 312 | 64.171 | 1.513 | 65.675 | 1.00 40.11 |
| ATOM · | 5499 5 5 00 | OE2 GLU B 312 | 63.539 65.358 | 0.614 1.782 | 65.081 65.437 | 1.00 43.69 1.00 39.26 |
| ATCM | 5501 | C GLU B 312 | 61.197 | 2.959 | 64.080 | 1.00 39.28 |
| | | ·= · - · - | ·-· | 2 | | |

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Figure 18-84

| ATOM | 5502 | 0 | .GLU E | 212 | 61.640 | 2.497 | 62 025 | 1 00 21 20 |
|--------------|--------------|----------|---------|-----------------|------------------|------------------|--------------------|--------------------------|
| MOTA | 5503 | | LEU E | | 59.919 | | 63.035 | 1.00 31.38 |
| | 5504 | | | | | | 64.438 | 1.00 26.70 |
| MOTA | 5505 | | | | 58.930 | | 63.598 | 1.00 26.73 |
| MOTA | 5506 | | | | 57.571 | | 64.297 | 1.00 25.83 |
| ATOM | | | | | 57.429 | 1.224 | 65.477 | 1.00 35.18 |
| MOTA | 5507 | | 1 LEU B | | 56.063 | 1.434 | 66.130 | 1.00 32.49 |
| MOTA | 5508 | | 2_LEU B | | 57.595 | -0.215 | 64.989 | 1.00 29.71 |
| ATOM | 5509 | С | LEU B | | 58.768 | 2.866 | | 1.00 29.03 |
| MOTA | 5510 | 0 | LEU B | | 58.716 | 2.187 | 61.228 | 1.00 25.39 |
| MOTA | 5511 | N | SER B | | 58.677 | 4.194 | 62.263 | 1.00 30.13 |
| MOTA | 5512 | CA | | - | 58.498 | 5.006 | 61.060 | 1.00 34.06 |
| MOTA | 5513 | CB | SER B | | 58.206 | 6.456 | 61.445 | 1.00 31.15 |
| ATOM | 5514 | OG | SER B | | 57.041 | 6.537 | 62.234 | 1.00 48.58 |
| MOTA | 5515 | С | SER B | | 59.707 | 5.003 | 60.151 | 1.00 31.84 |
| MOTA | 5516 | 0 | SER B | | 59.632 | 5.469 | 59.026 | 1.00 34.15 |
| ATOM | 5517 | N | GLY B | | 60.831 | 4.515 | 60.65 5 | 1.00 31.81 |
| MOTA | 5518 | CA | GLY B | | 62.036 | 4.485 | 59.848 | 1.00 37.27 |
| MOTA | 5519 | С | GLY B | | 62.659 | 5.851 | 59.616 | 1.00 39.93 |
| ATOM | 5520 | 0 | GLY B | | 63.363 | 6.054 | 58.624 | 1.00 39.79 |
| ATOM | 5521 | N | ARG B | | 62.422 | 6.798 | 60.518 | 1.00 38.22 |
| MOTA | 5522 | CA | ARG B | | 63.004 | 8.121 | 60.336 | 1.00 38.66 |
| ATOM | 5523 | CB | ARG B | | 61.908 | 9.184 | 60.275 | 1.00 40.20 |
| MOTA | 5524 | CG | ARG B | | 61.089 | 9.345 | 61.520 | 1.00 39.06 |
| MOTA | 5525 | CD | ARG B | | 60.032 | 10.398 | 61.284 | |
| ATOM | 5526 | NE | ARG B | | 59.002 | 9.954 | 60.352 | 1.00 45.09 |
| MOTA | 5527 | CZ | | 316 | 58.075 | 10.754 | 59.838 | 1.00 40.84 |
| MOTA | 5528 | NH] | | 316 | 58.064 | 12.033 | 60.170 | 1.00 48.44 |
| ATOM | 5529 | NH2 | | | 57.150 | 10.278 | 59.014 | 1.00 35.96 |
| ATOM | 5530 | C | ARG B | | 64.031 | 8.467 | 61.408 | 1.00 39.03 |
| MOTA | 5531 5532 | O | ARG B | | 63.952 | 7.988 | 62.539 | 1.00 34.34 |
| ATOM | 5533 | N CA | GLU B | | 65.003 | 9.296 | 61.035 | 1.00 39.58 |
| ATOM ATOM | 5534 | CB | GLU B | | 66.074 67.142 | 9.697 10.509 | 61.943 61.203 | 1.00 43.35 |
| ATOM | 5535 | CG | GLU B | | 67.609 | 9.910 | 59.884 | 1.00 49.34 1.00 57.04 |
| ATOM | 5536 | CD | GLU B | | 66.546 | 10.009 | 58.798 | 1.00 57.04 |
| ATOM | 5537 | OE1 | | | 66.146 | 11.149 | 58.467 | 1.00 62.79 |
| ATOM | 5538 | OE2 | | 317 | 66.108 | 8.954 | 58.280 | 1.00 64.46 |
| MOTA | 5539 | c | GLU B | | 65.555 | 10.528 | 63.100 | 1.00 41.58 |
| ATOM | 5540 | ō | GLU B | | 64.658 | 11.356 | 62.939 | 1.00 39.74 |
| ATOM | 5541 | N | VAL B | | 66.118 | 10.301 | 64.278 | 1.00 35.38 |
| MOTA | 5542 | CA | VAL B | | 65.706 | 11.049 | 65.448 | 1.00 38.76 |
| ATOM | 5543 | CB | VAL B | 318 | 66.000 | 10.265 | 66,750 | 1.00 42.28 |
| ATOM | 5544 | CG1 | VAL B | 318 | 65.560 | 11.080 | 67.962 | 1.00 38.26 |
| MOTA | 5545 | CG2 | VAL B. | 318 | 65.287 | 8.916 | 66.722 | 1.00 39.99 |
| ATOM | 5546 | C | VAL B | 318 | 66.459 | 12.370 | 65.478 | 1.00 41.82 |
| .TOM | 5547 | 0 | VAL B | 318 | 67.689 | 12.395. | 65.570 | 1.00 37.20 |
| ATOM | 5548 | N | PRO B | 319 | 65.735 | 13.491 | 65.356 | 1.00 43.18 |
| MOTa | 5549 | CD | PRO B | | 64.290 | 13.672 | 65.155 | 1.00 41.90 |
| MOTA | 5550 | CA | PRO B | | 66.402 | 14.792 | 65.388 | 1.00 44.31 |
| MOTA | 5551 | CB | PRO B | | 65.241 | 15.763 | 65.181 | 1.00 44.58 |
| ATOM | 5552 | CG | PRO B | | 64.079 | 15.011 | 65.795 | 1.00 43.34 |
| ATOM | 5553 | С | PRO B | | 67.086 | 14.965 | 66.741 | 1.00 44.62 |
| ATOM | 5554 | 0 | PRO B | | 66.541 | 14.565 | 67.771 | 1.00 43.75 |
| ATOM | .5555 | N | GLU B | | 68.277 | 15.552 | 66.735 | 1.00 44.16 |
| ATOM | 5556 | CA | GLU B | | 69.029 | 15.762 | 67.967 | 1.00 45.92 |
| MOTA | 5557 | CB | GLU B | | 70.381 | 16.406 | 67.663 | 1.00 50.87 |
| MOTA | 5558 | CG | GLU B | | 71.165 | 16.768 | 68.919 | 1.00 53.71 |
| MOTA | 5559 | CD | GLU B | | 72.455 | 17.505 | 68.620 | 1.00 57.75 |
| MOTA | 5560 | OE1 | GLU B | | 73.161 | 17.874 | 69.583 | 1.00 56.37 |
| MOTA | 5561 | OE2 | GLU B | | 72.762 | 17.714 | 67.427 | 1.00 60.07 |
| ATOM | 5562 | C | GLU B | | 68.311 | 16.625 | 68.995 | 1.00 44.42 |
| ATOM | 5563 | 0 | GLU B 3 | | 68.244 67.778 | 16.279 | 70.168 | 1.00 42.32 |
| ATOM | 5564 | N | LYS B 3 | | 67.778 | 17.753 | 68.550 | 1.00 42.50 |
| MOTA | 5565 5566 | CA | LYS B 3 | | 67.102 | 18.672 | 69.448 69.503 | 1.00 45.24 1.00 46.43 |
| MOTA | 5567 | CB CG | LYS B 3 | | 67.890 | 20.000 20.802 | 68.195 | 1.00 46.43 |
| MOTA | ,,,,,, | -6 | T10 D 3 | , T | 07.030 | 20.002 | | T.00 NT.43 |

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| ATOM | 5568 | CD LYS B 321 | 68.700 | 20.144 | 67.057 | 1.00 57.24 |
|-------------|------|----------------|--------|--------|--------|------------|
| ATOM | 5569 | CE LYS B 321 | 67.936 | 19.062 | 66.280 | 1.00 55.24 |
| MOTA | 5570 | | | 19.588 | 65.558 | 1.00 55.31 |
| | | | | | | |
| MOTA | 5571 | _ | | 18.971 | 69.098 | 1.00 43.44 |
| ATOM | 5572 | O LYS B 321 | 65.211 | 18.736 | 67.978 | 1.00 43.03 |
| ATOM | 5573 | N LEU B 322 | 64.947 | 19.512 | 70.076 | 1.00 39.45 |
| ATOM | 5574 | | | 19.885 | 69.875 | 1.00 40.31 |
| | | | | | | |
| ATOM | 5575 | | | 20.034 | 71.215 | 1.00 40.88 |
| MOTA | 5576 | CG LEU B 322 | 62.943 | 18.901 | 72.234 | 1.00 40.09 |
| ATOM | 5577 | CD1 LEU B 322 | 62.001 | 19.175 | 73.388 | 1.00 38.17 |
| ATOM | 5578 | | | 17.596 | 71.580 | 1.00 41:56 |
| | | | | | | |
| MOŢA | 5579 | _ | | 21.244 | 69.197 | 1.00 41.23 |
| ATOM | 5580 | O LEU B 322 | 64.466 | 22.070 | 69.531 | 1.00 39.22 |
| ATOM | 5581 | N ASN B 323 | 62.735 | 21.473 | 68.233 | 1.00 40.04 |
| | 5582 | CA ASN B 323 | 62.703 | 22.771 | 67.582 | 1.00 43.32 |
| ATOM | | | | | 66.234 | |
| . ATOM | 5583 | CB ASN B 323 | 61.985 | 22.707 | | 1.00 41.53 |
| ATOM | 5584 | CG ASN B 323 | 60.617 | 22.085 | 66.335 | 1.00 41.89 |
| ATOM | 5585 | OD1 ASN B 323 | 59.889 | 22.308 | 67.304 | 1.00 39.79 |
| ATOM | 5586 | ND2 ASN B 323 | 60.243 | 21.317 | 65.317 | 1.00 40.43 |
| | | | 61.949 | | 68.532 | 1.00 44.76 |
| "ATOM | 5587 | C ASN B 323 | | 23.690 | | |
| ATOM | 5588 | O ASN B 323 | 61.402 | 23.237 | 69.539 | 1.00 45.80 |
| MOTA | 5589 | N ASN B 324 | 61.902 | 24.973 | 68.210 | 1.00 46.85 |
| ATOM | 5590 | CA ASN B 324 | 61.234 | 25.930 | 69.076 | 1.00 47.60 |
| | 5591 | CB ASN B 324 | 61.460 | 27.348 | 68.549 | 1.00 50.87 |
| ATOM | | | | | | |
| ATOM | 5592 | CG ASN B 324 | 61.089 | 28.407 | 69.562 | 1.00 55.06 |
| ATOM | 5593 | OD1 ASN B 324 | 59.925 | 28.565 | 69.919 | 1.00 60.68 |
| ATOM | 5594 | ND2:ASN B 324 | 62.091 | 29.131 | 70.048 | 1.00 59.17 |
| ATOM | 5595 | C ASN B 324 | 59.740 | 25.664 | 69.249 | 1.00 43.97 |
| | 5596 | O ASN B 324 | 59.190 | 25.898 | 70.322 | 1.00 41.33 |
| ATOM | | | | | | |
| MOTA | 5597 | N LYS B 325 | 59.087 | 25.168 | 68.201 | 1.00 43.49 |
| ATOM | 5598 | CA LYS B 325 | 57.655 | 24.892 | 68.264 | 1.00 45.95 |
| ATOM | 5599 | CB LYS B 325 | 57.112 | 24.415 | 66.909 | 1.00 48.97 |
| ATOM | 5600 | CG LYS B 325 | 57.212 | 25.400 | 65.731 | 1.00 53.41 |
| | | | 58.582 | 25.386 | 65.024 | 1.00 58.77 |
| ATOM | 5601 | | | | | |
| MOTA | 5602 | CE LYS B 325 | 59.700 | 26.013 | 65.846 | 1.00 58.10 |
| ATOM | 5603 | NZ LYS B 325 | 61.024 | 25.906 | 65.178 | 1.00 53.38 |
| MOTA | 5604 | C LYS B 325 | 57.368 | 23.822 | 69.309 | 1.00 45.79 |
| | 5605 | O LYS B 325 | 56.375 | 23.891 | 70.034 | 1.00 43.91 |
| MOTA | | | | | 69.381 | 1.00 44.28 |
| ATOM | 5606 | N ALA B 326 | 58.245 | 22.829 | | |
| atom | 5607 | CA ALA B 326 | 58.078 | 21.746 | 70.336 | 1.00 44.25 |
| ATOM | 5608 | CB ALA B 326 | 59.013 | 20.589 | 69.986 | 1.00 41.44 |
| ATOM | 5609 | C ALA B 326 | 58.342 | 22.233 | 71.757 | 1.00 40.92 |
| ATOM | 5610 | O ALA B 326 | 57.639 | 21.843 | 72.688 | 1.00 39.02 |
| | | | | | 71.922 | 1.00 38.14 |
| ATOM | 5611 | N LYS B 327 | 59.352 | 23.085 | | |
| ATOM | 5612 | CA LYS B 327 | 59.689 | 23.603 | 73.246 | 1.00 40.11 |
| ATCM | 5613 | CB LYS B 32-7 | 60.892 | 24.552 | 73.178 | 1.00 42.36 |
| ATOM | 5614 | CG LYS B 327 | 62.174 | 23.922 | 72.(59 | 1.00 45.78 |
| | 5615 | CD LYS B 327 | 63.325 | 24.926 | 72.675 | 1.00 48.46 |
| ATOM | | | | | 72.031 | |
| ATOM | 5616 | CE LYS B 327 | 64.594 | 24.367 | | 1,00 49.62 |
| ATOM | 5617 | NZ . LYS B 327 | 65:108 | 23.139 | 72.700 | 1.00 48.53 |
| MOTA | 5618 | C LYS B 327 | 58.500 | 24.338 | 73.841 | 1.00 39.17 |
| | 5619 | O LYS B 327 | 58.132 | 24.112 | 74.994 | 1.00 38.87 |
| ATOM | | | | | 73.048 | 1.00 41.06 |
| atom | 5620 | N GLU B 328 | 57.898 | 25.215 | | |
| MOTA | 5621 | CA GLU B 328 | 56.750 | 25.986 | 73.512 | 1.00 42.35 |
| ATOM | 5622 | CB GLU B 328 | 56.357 | 27.028 | 72.463 | 1.00 44.02 |
| | 5623 | CG GLU B 328 | 57.434 | 28.084 | 72.258 | 1.00 44.80 |
| ATOM | | CD GLU B 328 | 57.835 | 28.742 | 73.569 | 1.00 48.40 |
| ATOM | 5624 | | | | 74.237 | |
| ATOM | 5625 | OE1 GLU B 328 | 56.949 | 29.317 | | 1.00 51.20 |
| ATOM | 5626 | OE2 GLU B 328 | 59.029 | 28.680 | 73.935 | 1.00 47.81 |
| ATOM | 5627 | C GLU B 328 | 55.569 | 25.087 | 73.839 | 1.00 38.67 |
| | 5628 | O GLU B 328 | 54.794 | 25.377 | 74.750 | 1.00 41.20 |
| atom | | | | _ | 73.090 | 1.00 35.31 |
| ATCM | 5629 | N LEU B 329 | 55.429 | 23.999 | | |
| ATOM | 5630 | CA LEU B 329 | 54.349 | 23.056 | 73.334 | 1.00 32.69 |
| ATCM. | 5631 | CB LEU B 329 | 54.404 | 21.900 | 72.334 | 1.00 35.06 |
| | 5632 | CG LEU B 329 | 53.344 | 20.813 | 72.544 | 1.00 35.01 |
| ATOM | | CD1 LEU B 329 | | 21.430 | 72.419 | 1.00 36.90 |
| ROTE | 5633 | HEU D 329 | 51.958 | 61.400 | | 30.20 |
| • | 4 | | | | | |

| MOTA | 5634 | CD | 2 LEU | B 329 | | 53.521 | 19.699 | 71.525 | 1.00 32.36 |
|--------|--------|-----|-------|---------|-----|--------|--------|--------|------------|
| MOTA | 5635 | | LEU | | | 54.504 | | 74.747 | 1.00 34.07 |
| MOTA | 5636 | | | B 329 | | 53.621 | 22.664 | 75.583 | 1.00 30.53 |
| ATOM | 5637 | | | B 330 | | 55.640 | 21.873 | 75.013 | 1.00 30.33 |
| | 5638 | | | B 330 | | 55.889 | | | |
| MOTA | | | | | | | 21.311 | 76.330 | 1.00 34.99 |
| ATOM | 5639 | | LEU | | | 57.267 | 20.642 | 76.382 | 1.00 37.01 |
| ATOM | 5640 | | LEU | | | 57.466 | 19.428 | 75.470 | 1.00 34.91 |
| ATOM | 5641 | | l LEU | | | 58.832 | 18.817 | 75.728 | 1.00 34.69 |
| ATOM | 5642 | CD: | | | | 56.369 | 18.396 | 75.742 | 1.00 34.10 |
| ATOM | 5643 | С | LEU | B 330 | | 55.789 | 22.363 | 77.429 | 1.00 37.12 |
| ATOM | 5644 | Q | LEU | B 330 | | 55.210 | 22.110 | 78.482 | 1.00 34.19 |
| ATOM | 5645 | N | LYS | B 331 | | 56.353 | 23.540 | 77.186 | 1.00 34.34 |
| ATOM | 5646 | CA | | B 331 | | 56.313 | 24.604 | 78.181 | 1.00 43.35 |
| ATOM | 5647 | СВ | | B 331 | | 57.162 | 25.788 | 77.712 | 1.00 46.25 |
| ATOM | 5648 | CG | | B 331 | | 58.658 | 25.496 | 77.685 | 1.00 51.07 |
| ATOM | 5649 | CD | | B 331 | | 59.482 | | | |
| | 5650 | CE | | | | | 26.610 | 77.021 | 1.00 49.96 |
| ATOM | | | | B 331 | | 59.371 | 27.957 | 77.733 | 1.00 53.08 |
| ATOM | 5651 | NZ | | B 331 | | 58.013 | 28.569 | 77.662 | 1.00 56.18 |
| MOTA | 5652 | С | | B 331 | | 54.892 | 25.069 | 78.494 | 1.00 42.06 |
| MOTA | 5653 | Ο. | | B 331 | | 54.588 | 25.416 | 79.631 | 1.00 43.05 |
| ATOM | 5654 | N | | B 332 | | 54.018 | 25.056 | 77.492 | 1.00 44.54 |
| ATOM | 5655 | CA | SER | B 332 | | 52.639 | 25.502 | 77.679 | 1.00 46.58 |
| ATOM | 5656 | CB | SER | B 332 | | 51.975 | 25.751 | 76.329 | 1.00 48.75 |
| ATOM | 5657 | OG | SER | B 332 | | 51.769 | 24.527 | 75.646 | 1.00 49.55 |
| ATOM | 5658 | C | SER | B 332 | | 51.780 | 24.507 | 78.451 | 1.00 49.56 |
| ATOM | 5659 | o | | B 332 | | 50.618 | 24.791 | 78.749 | |
| ATOM | 5660 | N | | | • . | 52.341 | 23.345 | 78.770 | 1.00 50.55 |
| ATOM | 5661 | CA | ILE | | • . | 51.586 | 22.326 | 79.488 | 1.00 51.93 |
| ATOM | 5662 | CB | ILE | | | 52.259 | 20.945 | 79.376 | 1.00 51.82 |
| ATOM | 5663 | CG2 | | | | 51.447 | 19.902 | 80.134 | 1.00 50.29 |
| | 5664 | CG1 | | | | 52.359 | 20.539 | 77.905 | |
| ATOM | | CD1 | | B 333 | | | | | 1.00 52.18 |
| ATOM | 5665 | | | | | 53.044 | 19.210 | 77.693 | 1.00 55.42 |
| MOTA | 5666 | C | | B 333 | , | 51.367 | 22.634 | 80.964 | 1.00 51.45 |
| ATOM | 5667 | 0 | | B 333 - | | 52.180 | 23.290 | 81.614 | 1.00 50.96 |
| ATOM | 5668 | N | | B 334 | | 50.245 | 22.141 | 81.472 | 1.00 54.05 |
| ATOM | 5669 | CA | | B 334 | | 49.850 | 22.306 | 82.865 | 1.00 58.15 |
| ATOM | 5670 | CB | | B 334 | | 48.320 | 22.216 | 82.959 | 1.00 60.38 |
| ATOM | . 5671 | CG | | B 334 | | 47.751 | 20.972 | 82.262 | 1.00 63.85 |
| ATOM | 5672 | OD1 | ASP | B 334 | | 48.017 | 19.833 | 82.710 | 1.00 59.16 |
| ATOM | 5673 | OD2 | ASP | B 334 | | 47.033 | 21.138 | 81.252 | 1.00 59.71 |
| ATOM | 5674 | С | ASP | B 334 | | 50.506 | 21.207 | 83.701 | 1.00 55.47 |
| MOTA | 5675 | 0 | ASP | B 334 | | 49.833 | 20.291 | 84.171 | 1.00 54.08 |
| ATOM | 5676 | N | | B 335 | | 51.816 | 21.307 | 83.906 | 1.00 54.60 |
| MOTA | 5677 | CA | | B 335 | | 52.524 | 20.266 | 84.641 | 1.00 56.60 |
| ATOM | 5678 | CB | | B 335 | | 53.718 | 19.784 | 83.811 | 1.00 53.01 |
| ATOM | 5679 | CG | | B 335 | | 54.522 | 18.717 | 84.482 | 1.00 49.30 |
| MOTA | 5686 | | | B 335 | | 53.898 | 17.589 | 85.008 | 1.00 45.61 |
| ATOM | 5681 | | PHE | | | 55.901 | 18.843 | 84.605 | 1.00 46.83 |
| | 5682 | | PHE | | | | | 85.651 | _ |
| ATOM | | CE1 | | | | 54.637 | 16.600 | | |
| MOTA | 5683 | | | B 335 | | 56.651 | 17.860 | 85.247 | 1.00 46.02 |
| MOTA | 5684 | CZ | | B 335 | | 56.018 | 16.737 | 85.772 | 1.00 46.08 |
| ATOM | 5685 | С | | B 335 | | 52.971 | 20.559 | 86.072 | 1.00 57.29 |
| ATOM | 5686 | 0 | | B 335 | | 52.197 | 20.378 | 87.012 | 1.00 63.54 |
| ATOM | 5687 | N | GLU 1 | B 336 | | 54.223 | 20.983 | 86.229 | 1.00 55.21 |
| MOTA | 5688 | CA | GLU 1 | B 336 | | 54.818 | 21.286 | 87.535 | 1.00 60.30 |
| MOTA | 5689 | CB | GLU ! | 336 | | 53.783 | 21.846 | 88.517 | 1.00 64.95 |
| ATOM | 5690 | CG | GLU I | B 336 | | 54.375 | 22.225 | 89.867 | 1.00 71.50 |
| ATOM | 5691 | CD | | B 336 | | 53.363 | 22.882 | 90.787 | 1.00 75.37 |
| ATOM | 5692 | | | B 336 | | 52.796 | 23.925 | 90.394 | 1.00 75.32 |
| ATOM | 5693 | | GLU I | | | 53.137 | 22.361 | 91.901 | 1.00 76.84 |
| ATOM | 5694 | C | GLU I | | | 55.485 | 20.058 | 88.146 | 1.00 55.66 |
| ATOM | 5695 | | GLU I | | | 54.823 | 19.093 | 88.529 | 1.00 33.00 |
| | | | GLU E | | | • | | 88.240 | 1.00 54.26 |
| ATOM | 5696 | | | | | 56.807 | 20.125 | | |
| ATOM · | 5697 | | GLU I | | | 57.630 | 19.047 | 88.767 | 1.00 54.35 |
| ATOM | 5698 | _ | GLU E | | | 59.101 | 19.457 | 88.635 | 1.00 54.08 |
| ATOM | 5699 | CG | GLU I | 3 337 | | 60.074 | 18.315 | 88.514 | 1.00 54.15 |

| | | | J | | | |
|--------------|---------------|--------------------------------|------------------|------------------|------------------|--------------------------|
| ATOM | 5700 | CD GLU B 337 | 59.856 | 17.496 | 87.259 | 1.00 48.94 |
| MOTA | 5701 | | 59.958 | | 86.142 | 1.00 41.06 |
| MOTA | 5702 | | 59.581 | | 87.391 | 1.00 50.23 |
| ATOM ATOM | 5703 5704 | | 57.278 57.130 | 18.740 19.651 | 90.227 | 1.00 55.08 |
| ATOM | 5705 | | 57.130 | 17.458 | 91.039 90.557 | 1.00 54.51 1.00 56.20 |
| MOTA | 5706 | | 56.798 | 17.048 | 91.918 | 1.00 57.73 |
| MOTA | 5707 | | 56.713 | 15.527 | 92.020 | 1.00 58.47 |
| ATOM | 5708 | | 56.231 | 15.034 | 93.359 | 1.00 63.17 |
| MOTA MOTA | 5709 5710 | | 54.882 | 15.096 | 93.696 | 1.00 64.86 |
| ATOM | 5711 | | 57.129 54.434 | 14.526 14.656 | 94.293 94.943 | 1.00 63.51 1.00 65.25 |
| ATOM | 5712 | | 56.693 | 14.087 | 95.539 | 1.00 63.23 |
| MOTA | 5713 | | 55.342 | 14.152 | 95.864 | 1.00 66.30 |
| MOTA | 5714 | C PHE B 338 | 57.836 | 17.539 | 92.918 | 1.00 61.85 |
| MOTA MOTA | 5715 5716 | O PHE B 338 N ASP B 339 | 57.520 59.081 | 17.807 | 94.078 | 1.00 58.15 |
| MOTA | 5717 | CA ASP B 339 | 60.167 | 17.636 18.099 | 92.466 93.316 | 1.00 64.63 1.00 67.53 |
| MOTA | 5718 | CB ASP B 339 | 61.286 | 17.059 | 93.362 | 1.00 67.33 |
| ATOM · | 5719 | CG ASP B 339 | 62.474 | 17.524 | | 1.00 68.13 |
| ATOM | 5720 | OD1 ASP B 339 | 62.280 | 17.909 | 95.346 | 1.00 68.68 |
| ATOM ATOM | 5721 5722 | OD2 ASP B 339 C ASP B 339 | 63.603 | 17.502 | 93.646 | 1.00 69.03 |
| ATOM | 5723 | O ASP B 339 | 60.718 61.211 | 19.435 19.545 | 92.829 91.708 | 1.00 69.03 1.00 67.54 |
| ATOM | 5724 | N ASP B 340 | 60.626 | 20.442 | 93.693 | 1.00 67.34 |
| MOTA | 5725 | CA ASP B 340 | 61.088 | 21.797 | 93.402 | 1.00 75.20 |
| ATOM | 5726 | CB ASP B 340 | 61.113 | 22.623 | 94.689 | 1.00 77.04 |
| MOTA MOTA | 5727 5728 | CG ASP B 340 OD1 ASP B 340 | 59.766 58.803 | 22.671 23.181 | 95.375 94.763 | 1.00 78.70 |
| ATOM | 5729 | OD2 ASP B 340 | 59.668 | 22.194 | 96.525 | 1.00 79.66 1.00 80.53 |
| MOTA | 5730 | C ASP B 340 | 62.464 | 21.856 | 92.751 | 1.00 74.82 |
| MOTA | 5731 | O ASP B 340 | 62.615 | 22.400 | 91.659 | 1.00 78.48 |
| ATOM ATOM | 5732 5733 | N GLU B 341 CA GLU B 341 | 63.465 | 21.303 | 93.426 | 1.00 74.11 |
| ATOM | 5734 | CB GLU B 341 | 64.827 65.818 | 21.312 21.596 | 92.907 94.040 | 1.00 76.25 1.00 79.54 |
| ATOM | 5735 | CG GLU B 341 | 67.277 | 21.653 | 93.596 | 1.00 82.33 |
| MOTA | 5736 | CD GLU B 341 | 67.539 | 22.750 | 92.577 | 1.00 83.24 |
| ATOM | 5737 5738 | OE1 GLU B 341 OE2 GLU B 341 | 67.333 | 23.937 | 92.910 | 1.00 85.25 |
| ATOM ATOM | 57 3 9 | C GLU B 341 | 67.950 65.196 | 22.427 19.998 | 91.443 92.227 | 1.00 83.72 1.00 73.97 |
| ATOM | 5740 | O GLU B 341 | 65.627 | 19.051 | 92.883 | 1.00 77.10 |
| ATOM | 5741 | N VAL B 342 | 65.033 | 19.946 | 90.910 | 1.00 71.92 |
| MOTA | 5742 | CA VAL B 342 | 65.354 | 18.744 | 90.151 | 1.00 68.51 |
| MOTA MOTA | 5743 5744 | CB VAL B 342 CG1 VAL B 342 | 64.081 63.268 | 18.027 17.552 | 89.663 90.837 | 1.00 68.83 1.00 67.57 |
| ATOM | 5745 | CG2 VAL B 342 | 63.255 | 18.969 | 88.806 | 1.00 67.72 |
| ATOM | 5746 | C VAL B 342 | 66.201 | 19.059 | 88.927 | 1.00 65 35 |
| ATOM | 5747 | O VAL B 342 | 67.177 | 18.366 | 88.640 | 1.00 68.31 |
| MOTA MOTA | 5748 5749 | N ASP'B 343 CA ASP B 343 | 65.819 | 20.112 | 88.213 | 1.00 60.89 |
| ATOM | 5750 | CB ASP B 343 | 66.514 68.024 | 20.520 20.636 | 86.998 87.223 | 1.00 58.89 1.00 63.48 |
| ATOM | 5751 | CG ASP B 343 | 68.763 | 21.070 | 85.966 | 1.00 66.69 |
| ATOM | 5752 | OD1 ASP B 343 | 70.012 | 21.070 | 85.970 | 1.00 67.64 |
| ATOM | 5753 | OD2 ASP B 343 | 68.089 | 21.420 | 84.973 | 1.00 65.42 |
| MOTA | 5754 5755 | C ASP B 343 O ASP B 343 | 66.264 66.993 | 19.499 | 85.900 85.766 | 1.00 53.17 |
| ATOM ATOM | 5756 | N ARG B 344 | 65.216 | 18.516 19.735 | 85.124 | 1.00 49.70 1.00 50.24 |
| MOTA | 5757 | CA ARG B 344 | 64.868 | 18.853 | 84.022 | 1.00 46.49 |
| ATOM | 5758 | CB ARG B 344 | 63.467 | 18.269 | 84.228 | 1.00 42.41 |
| MOTA | 5759 | CG ARG B 344 | 63.317 | 17.367 | 85.452 | 1.00 38.59 |
| MOTA | 5760 5761 | CD ARG B 344 NE ARG B 344 | 64.344 64.169 | 16.246 | 85.432 86.537 | 1.00 37.12 |
| atom Mota | 5762 | CZ ARG B 344 | 65.078 | 15.310 14.413 | 86.905 | 1.00 36.55 1.00 37.20 |
| ATOM | 5763 | NH1 ARG B 344 | 66.234 | 14.331 | 86.259 | 1.00 33.53 |
| ATOM | 5764 | NH2 ARG B 344 | 64.830 | 13.595 | 87.915 | 1.00 28.79 |
| MOTA | 5765 | C ARG B 344 | 64.910 | 19.660 | 82.732 | 1.00 44.45 |

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Figure 18-88

| ATOM | 576 | 6 O ARG B 344 | 64.328 | 19.269 | 81.720 | 1.00 38.73 |
|--------------|--------------|----------------------------|------------------|------------------|------------------|--------------------------|
| ATOM | 576 | | 65.618 | | | |
| ATOM | 5768 | 8 CA SER B 345 | 65.740 | | | |
| MOTA | 5769 | 5 343 | 66.661 | | | |
| ATOM | 5770 | | 67.956 | | | |
| ATOM | | | 66.244 | 20.981 | | |
| MOTA | 577,2 | | 65.840 | 21.333 | | |
| ATOM | 5773 | | 67.117 | 19.992 | 80.534 | 1.00 33.93 |
| ATOM | 5774 | | 67.661 | 19.264 | 79.391 | 1.00 34.77 |
| ATOM | 5775 | | 68.660 | 18.206 | 79.877 | 1.00 36.09 |
| ATOM | 5776 | | 68.054 | 17.146 | 80.774 | 1.00 34.27 |
| MOTA | 5777 | | 67.433 | 16.013 | 80.240 | 1.00 37.62 |
| MOTA | 5778 | | 66.843 | 15.048 | 81.077 | 1.00 36.73 |
| ATOM ATOM | 5779 5780 | | 68.072 | 17.294 | 82.157 | 1.00 36.40 |
| ATOM | 5781 | | 67.489 | 16.344 | 82.999 | 1.00 36.54 |
| ATOM | 5782 | | 66.878 | 15.228 | 82.457 | 1.00 36.54 |
| ATOM | 5783 | | 66.310 | 14.306 | 83.306 | 1.00 33.35 |
| ATOM | 5784 | | 66.563 | 18.599 | 78.570 | 1.00 36.26 |
| ATOM | 5785 | | 66.719 65.445 | 18.385 | 77.367 | 1.00 40.50 |
| ATOM | 5786 | | 64.346 | 18.282 | 79.214 | 1.00 32.72 |
| ATOM | 5787 | | | 17.628 17.164 | 78.516 | 1.00 35.43 |
| MOTA | 5788 | | 63.819 | 16.292 | 79.513 80.635 | 1.00 34.36 1.00 28.32 |
| ATOM | 5789 | SD MET B 347 | 62.515 | 15.604 | 81.669 | 1.00 28.32 |
| ATOM | 5790 | CE MET B 347 | 61.654 | 17.027 | 82.142 | 1.00 34.47 |
| MOTA | 5791 | C MET B 347 | 63.701 | 18.525 | 77.465 | 1.00 39.04 |
| ATOM | 5792 | O MET B 347 | 63.060 | 18.029 | 76.540 | 1.00 37.38 |
| ATOM | 5793 | N LEU B 348 | 63.857 | 19.839 | 77.606 | 1.00 39.21 |
| MOTA | 5794 | CA LEU B 348 | 63.272 | 20.773 | 76.645 | 1.00 40.81 |
| MOTA | 5795 | CB LEU B 348 | 62.806 | 22.058 | 77.339 | 1.00 36.87 |
| MOTA | 5796 | CG LEU B 348 | 61.690 | 21.975 | 78.384 | 1.00 42.66 |
| MOTA | 5797 5798 | CD1 LEU B 348 | 61.507 | 23.337 | 79.032 | 1.00 43.41 |
| ATOM | 5799 | CD2 LEU B 348 | 60.391 | 21.511 | 77.741 | 1.00 40.47 |
| MOTA MOTA | 5800 | C LEU B 348 O LEU B 348 | 64.289 | 21,133 | 75.573 | 1.00 41.13 |
| ATOM | 5801 | N GLU B 349 | 64.018 | 21.968 | 74.711 | 1.00 38.93 |
| ATOM | 5802 | CA GLU B 349 | 65.455 66.527 | 20.495 | 75.632 | 1.00 37.70 |
| ATOM | 5803 | CB GLU B 349 | 67.856 | 20.757 20.953 | 74.681 75.422 | 1.00 42.48 |
| ATOM | 5804 | CG GLU B 349 | 67.834 | 22.035 | 76.493 | 1.00 45.02 1.00 53.82 |
| MOTA | 5805 | CD GLU B 349 | 67.483 | 23.402 | 75.938 | 1.00 57.46 |
| MOTA | 5806 | OE1 GLU B 349 | 68.211 | 23.885 | 75.044 | 1.00 59.62 |
| MOTA | 5807 | OE2 GLU B 349 | 66.480 | 23.993 | 76.397 | 1.00 57.91 |
| MOTA | 5808 | C GLU B 349 | 66.709 | 19.638 | 73.664 | 1.00 43.57 |
| MOTA | 5809 | O GLU B 349 | 66.577 | 19.849 | 72.459 | 1.00 41.26 |
| ATOM | 5810 | N THR B 350 | 67.02 7 | 18.448 | 74.161 | 1.00 41.95 |
| MOTA | 5811 | CA THR B 350 | 67.264 | 17.299 | 73.298 | 1.00 40.02 |
| ATOM | 5812 | CB THR B 350 | 68.689 | 16.775 | 73.504 | 1.00 43.08 |
| ATOM | 5813 | OG1 THR B 350 | 68.894 | 16.490 | 74.894 | 1.00 41.07 |
| ATOM . | 5814 5815 | CG2 THR B 350 | 69.703 | 17.816 | 73.049 | 1.00 45.05 |
| ATOM | 5816 | C THR B 350 O THR B 350 | 66.278 | 16.154 | 73.510 | 1.00 37.56 |
| MOTA | 5817 | N LEU B 351 | 65.754 66.043 | 15.966 | 74.611 | |
| ATOM | 5818 | CA LEU B 351 | 65.126 | 15.391 | 72.445 | 1.00 32.86 |
| ATOM | 5819 | CB LEU B 351 | 64.776 | 14.260 13.810 | 72.475 | 1.00 35.00 |
| ATOM | 5820 | CG LEU B 351 | 63.709 | 14.601 | 71.053 70.312 | 1.00 31.61 |
| ATOM | 5821 | CD1 LEU B 351 | 63.552 | 14.064 | 68.904 | 1.00 35.31 1.00 37.88 |
| ATOM | 5822 | CD2 LEU B 351 | 62.397 | 14.474 | 71.068 | 1.00 39.36 |
| MOTA | 5823 | C LEU B 351 | 65.662 | 13.065 | 73.240 | 1.00 33.33 |
| MOTA | 5824 | O LEU B 351 | | 12.469 | 74.046 | 1.00 31.48 |
| ATOM | 5825 | N LYS B 352 | | 12.720 | 72.981 | 1.00 29.58 |
| ATOM | 5826 | CA LYS B 352 | | 11.576 | 73.633 | 1.00 36.77 |
| ATOM | 5827 | CB LYS B 352 | | 10.864 | 72.647. | 1.00 34.32 |
| ATOM . | 5828 | CG LYS B 352 | | 10.563 | 71.326 | 1.00 39.29 |
| MOTA | 5829 | CD LYS B 352 | 68.703 | 9.949 | 70.294 | 1.00 42.25 |
| ATOM | 5830 | CE LYS B 352 | 69.110 | 8.541 | 70.655 | 1.00 46.22 |
| MOTA | 5831 | NZ LYS B 352 | 69.831 | 7.905 | 69.516 | 1.00 44.15 |
| | | | | | • | |

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Figure 18-89

| ATOM | 583 | C LYS B 352 | 6 | 8.295 | 11.983 | 74.878 | 1.00 | 36.30 |
|--------------|--------------|-----------------------------|-----|--------------|------------------|------------------|------|----------------|
| ATOM | 583 | 3 O LYS B 352 | 6. | 9.086 | 12.931 | _ | 1.00 | |
| ATOM | 5834 | | 6 | 8.049 | 11.275 | 75.967 | 1.00 | 30.01 |
| MOTA | 583 | | 6 | 3.757 | 11.569 | | | 33.99 |
| ATOM | 5836 | | 6 | 7.852 | 11.308 | | | 38.57 |
| MOTA | 5837 | | | 7.134 | 9.986 | 78.315 | 1.00 | 43.90 |
| ATOM | 5838 | | | 5.034 | 9.851 | 78.926 | 1.00 | 22.39 |
| MOTA | 5839 | | | 7.679 | 9.078 | 77.649 | 1.00 | 50.42 |
| ATOM | 5840 | | | 0.022 | 10.723 | 77.202 | 1.00 | 35.83 |
| ATOM | 5841 | | |).189 | 9.833 | 76.368 | | 23.71 |
| ATOM | 5842 | | |).954 | 11.025 | 78.116 | | 36.36 |
| MOTA | 5843 | | | .928 | 12.093 | 79.132 | | 38.28 |
| MOTA | 5844 5845 | | | .205 | 10.277 | 78.212 | | 33.62 |
| MOTA MOTA | 5846 | | 73 | .003 | 11.104 | 79.213 | | 34.46 |
| ATOM | 5847 | | | .924 | 11.556 | 80.164 | | 38.08 |
| ATOM | 5848 | • | | .894 | 8.883 8.643 | 78.733 79.366 | | 33.62 |
| ATOM | 5849 | | | .833 | 7.954 | 78.468 | | 24.82 31.76 |
| ATOM | 5850 | | 72 | .635 | 6.611 | 78.969 | | 30.01 |
| ATOM | 5851 | | | .653 | 5.655 | 78.359 | | 34.02 |
| ATOM | 5852 | | | .025 | 4.378 | 77.910 | | 44.37 |
| ATOM | 5853 | CD2 TRP B 355 | | .263 | 3.072 | 78.436 | | 45.39 |
| MOTA | 5854 | CE2 TRP B 355 | | .418 | 2.177 | 77.734 | | 44.31 |
| MOTA | 5855 | CE3 TRP B 355 | | .107 | 2.569 | 79.432 | | 47.19 |
| ATOM | 5856 | CD1 TRP B 355 | 72 | .073 | 4.230 | 76.935 | | 42.18 |
| ATOM | 5857 | NE1 TRP B 355 | 71 | .704 | 2.910 | 76.826 | | 37.84 |
| ATOM | 5858 | CZ2 TRP B 355 | | .395 | 0.808 | 77.999 | 1.00 | 44.97 |
| MOTA | 5859 | CZ3 TRP B 355 | | .084 | 1.207 | 79.694 | | 50.83 |
| ATOM | 5860 | CH2 TRP B 355 | | .231 | 0.341 | 78.979 | | 48.73 |
| MOTA | 5861 | C TRP B 355 | | .819 | 6.685 | 80.485 | | 30.87 |
| MOTA | 5862 5863 | O TRP B 355 | | .622 | 7.474 | 80.981 | | 26.93 |
| ATOM | 5864 | N ARG B 356 CA ARG B 356 | 72 | .061 .147 | 5.880 | 81.218 | | 24.96 |
| ATOM ATOM | 5865 | CB ARG B 356 | | .811 | 5,848 | 82.671 | | 23.57 |
| ATOM | 5866 | CG ARG B 356 | | .534 | 6:319 7.795 | 83.257 82.941 | | 24.71 23.66 |
| ATOM | 5867 | CD ARG B 356 | | .067 | 8.212 | 83.055 | | 20.14 |
| ATOM | 5868 | NE ARG B 356 | | .926 | 9.610 | 82.642 | | 20.59 |
| ATOM | 5869 | CZ ARG B 356 | | 787 | 10.192 | 82.288 | | 25.41 |
| ATOM | 5870 | NH1 ARG B 356 | | 644 | 9.508 | 82.287 | | 17.01 |
| ATOM | 5871 | NH2 ARG B 356 | 67. | 796 | 11.464 | 81.910 | | 20.07 |
| MOTA | 5872 | C ARG B 356 | 72. | 481 | 4.410 | 83.085 | | 26.57 |
| ATOM | 5873 | O ARG B 356 | | 610 | 3.641 | 83.485 | 1.00 | 23.02 |
| ATOM | 5874 | N GLY B 357 | | 761 | 4.063 | 82.978 | | 23.92 |
| ATOM | 5875 | CA GLY B 357 | | 186 | 2.712 | 83.294 | | 25.54 |
| ATOM | 5876 | C GLY B 357 | | 796 | 2.464 | 84.657 | | 24.35 |
| ATOM | 5877 5878 | O GLY B 357 N GLY B 358 | | 523. | 3.161 | 85.628 | | 25.88 |
| ATCM | 5879 | N GLY B 358 CA GLY B 358 | | 638 | 1.444 | 84.718 | | 24.32 |
| ATOM ATOM | 5880 | C GLY B 358 | | 282 412 | 1.070 | 85.960 | | 23.56 |
| ATOM | 5881 | 0 GLY B 358 | | 146 | -0.441 -1.051 | 85.924 84.889 | | 29.26 |
| ATOM | 5882 | N GLU B 359 | | 814 | -1.051 | 87.033 | | 23.71 27.64 |
| ATOM | 5883 | CA GLU B 359 | | 955 | ~2.503 | 87.078 | | 32.15 |
| ATOM | 5884 | CB GLU B 359 | | 822 | -2.936 | 88.265 | 1.00 | |
| ATOM | 5885 | CG GLU B 359 | | 125 | -2.772 | 89.601 | 1.00 | |
| ATOM | 5886 | CD GLU B 359 | 77. | | -3.479 | 90.741 | 1.00 | |
| ATCM | 5887 | OE1 GLU B 359 | 77. | | ~3.521 | 91.861 | 1.00 | |
| ATOM | 5888 | OE2 GLU B 359 | 78. | | -3.990 | 90.520 | 1.00 | |
| ATOM | 5889 | C GLU B 359 | 75. | | -3.122 | 87.261 | 1.00 | |
| ATOM | 5890 | O GLU B 359 | 74. | 612 | -2.429 | 87.588 | 1.00 | |
| ATCM | 5891 | N VAL B 360 | 75. | 482 | -4.428 | 87.053 | 1.00 | |
| ATCM | 5892 | CA VAL B 360 | 74. | | -5.147 | 87.251 | 1.00 | |
| ATOM | 5893 | CB VAL B 360 | 74. | | -6.270 | 86.200 | 1.00 | |
| ATOM | 5894 | CG1 VAL B 360 | 72. | | -7.045 | 86.492 | 1.00 | |
| ATOM | 5895 | CG2 VAL B 360 | 73. | 969 | -5.670 | 84.796 | 1.00 | |
| ATOM | 5896 | C VAL B 360 | 74. | | ~5.784 | 88.625 | 1.00 | |
| ATCM | 5897 | O VAL B 360 | 75. | 150 | -6.693 | 88.821 | 1.00 | 27,55 |

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Figure 18-90

| MOTA | 5898 | N ARG B 361 | 73.553 | -5.289 | 89.575 | 1.00 26.45 |
|--------|------|--|-------------------|--------|--------|------------|
| ATOM | 5899 | | | | | |
| | | | | -5.821 | 90.935 | 1.00 28.47 |
| ATOM | 5900 | CB ARG B 361 | 72.479 | -5.146 | 91.787 | 1.00 30.55 |
| ATOM | 5901 | CG ARG B 361 | 72.937 | -3.877 | 92.485 | 1.00 32.61 |
| ATOM | 5902 | | · | -3.163 | 93.117 | 1.00 35.00 |
| | | | | | | |
| ATOM | 5903 | | | -2.617 | 92.094 | 1.00 30.31 |
| ATOM | 5904 | CZ ARG B 361 | 69.753 | -1.925 | 92.350 | 1.00 29.45 |
| ATOM | 5905 | NH1 ARG B 361 | 69.385 | -1.689 | 93.605 | 1.00 18.49 |
| ATOM | 5906 | | | -1.428 | 91.348 | 1.00 30.49 |
| | | | • | | | |
| MOTA | 5907 | | | -7.322 | 91.001 | 1.00 30.17 |
| MOTA | 5908 | O ARG B 361 | 72.665 | -7.910 | 90.168 | 1.00 23.60 |
| MOTA | 5909 | N LYS B 362 | 73.949 | -7.922 | 92.022 | 1.00 33.09 |
| MOTA | 5910 | | | -9.351 | 92.272 | 1.00 36.94 |
| | | | | | | |
| MOTA | 5911 | CB LYS B 362 | | -9.706 | 93.513 | 1.00 40.24 |
| ATOM | 5912 | CG LYS B 362 | 76.190 | -9.527 | 93.337 | 1.00 52.55 |
| ATOM | 5913 | CD LYS B 362 | 76.571 | -8.126 | 92.849 | 1.00 56.65 |
| ATOM | 5914 | CE LYS B 362 | | -7.032 | 93.819 | 1.00 53.39 |
| | 5915 | NZ LYS B 362 | | | | |
| ATOM | | | | -5.680 | 93.341 | 1.00 48.87 |
| MOTA | 5916 | C LYS B 362 | 72.427 | -9.826 | 92.463 | 1.00 32.84 |
| MOTA | 5917 | O LYS B 362 | 72.045 - | 10.867 | 91.938 | 1.00 28.27 |
| ATOM | 5918 | N GLU B 363 | | -9.075 | 93.215 | 1.00 34.67 |
| | 5919 | CA GLU B 363 | | | 93.435 | 1.00 35.72 |
| MOTA | | and the second s | | -9.493 | | |
| ATOM | 5920 | CB GLU B 363 | | -8.532 | 94.390 | 1.00 36.04 |
| ATOM | 5921 | CG GLU B 363 | 69.502 | -7.077 | 93.977 | 1.00 44.81 |
| ATOM | 5922 | CD GLU B 363 | 68.859 | -6.186 | 95.033 | 1.00 52.14 |
| ATOM | 5923 | OE1 GLU B 363 | | -6.370 | 95.341 | |
| | | | | | | |
| ATOM | 5924 | | | -5.300 | 95.566 | 1.00 57.31 |
| ATOM | 5925 | C GLU B 363 | 69.501 | -9.619 | 92.111 | 1.00 30.68 |
| ATOM | 5926 | O GLU B 363 | 68.695 -: | 10.530 | 91.944 | 1.00 30.45 |
| MOTA | 5927 | N VAL B 364 | 69.784 | -8.724 | 91.166 | 1.00 26.19 |
| ATOM | 5928 | CA VAL B 364 | | -8.789 | 89.852 | 1.00 24.65 |
| | | | | | | |
| MOTA | 5929 | CB VAL B 364 | | -7.599 | 88.958 | 1.00 23.49 |
| ATOM | 5930 | CG1 VAL B 364 | 68.924 | -7.770 | 87.563 | 1.00 21.01 |
| ATOM | 5931 | CG2 VAL B 364 | 69.049 - | -6.293 | 89.587 | 1.00 23.08 |
| ATOM | 5932 | C VAL B 364 | 69.530 - | | 89.144 | 1.00 23.19 |
| | 5933 | O VAL B 364 | 68.691 - | | 88.542 | 1.00 23.06 |
| MOTA | | | | | | |
| ATOM | 5934 | N LYS B 365 | 70.810 - | | 89.216 | 1.00 27.15 |
| ATOM | 5935 | CA LYS B 365 | 71.296 - | 11.668 | 88.594 | 1.00 29.18 |
| ATOM | 5936 | CB LYS B 365 | 72.821 -1 | 11.758 | 88.704 | 1.00 28.61 |
| ATOM | 5937 | CG LYS B 365 | 73.554 -1 | | 88.030 | 1.00 30.27 |
| | | | | | | |
| ATOM | 5938 | | 75.074 -1 | | 88.154 | 1.00 32.58 |
| MOTA | 5939 | CE LYS B 365 | | -9.587 | 87.516 | 1.00 29.13 |
| MOTA | 5940 | NZ LYS B 365 | 77.271 - | -9.689 | 87.606 | 1.00 35.17 |
| MOTA | 5941 | C LYS B 365 | 70.666 -3 | 12.879 | 89.276 | 1.00 25.30 |
| ATOM | 5942 | O LYS B 365 | 70.282 -1 | | 88613 | 1.00 26.81 |
| | | | | | | 1.00 26.10 |
| ATOM | 5943 | | 70 559 -1 | | 90.604 | |
| ATOM | 5944 | CA ASP B 366 | 69 963 -1 | | 91.347 | 1.00 28.29 |
| ATOM | 5945 | CB ASP B 366 | 70.105 -1 | 13.731 | 92.859 | 1.00 29.44 |
| MOTA | 5946 | CG ASP B 366 | 71.557 -1 | 13.669 | 93.311 | 1.00 32.95 |
| ATOM | 5947 | OD1 ASP B 366 | 72.446 -1 | | 92.551 | 1.00 26.37 |
| | - | OD2 ASP B 366 | | | | |
| MOTA | 5948 | | 71.811 -1 | | 94.442 | 1.00 35.26 |
| MOTA | 5949 | C ASP B 366 | 68.487 -1 | 4.110 | 90.986 | 1.00 28.61 |
| MOTA | 5950 | O ASP B 366 | 68.000 -1 | 15.231 | 90.869 | 1.00 27.00 |
| ATOM | 5951 | N THR B 367 | 67.777 -1 | | 90.801 | 1.00 28.63 |
| | | | | | | 1.00 27.35 |
| MOTA | 5952 | CA THR B 367 | 66.365 -1 | | 90.438 | |
| ATOM | 5953 | CB THR B 367 | 65.726 -1 | | 90.359 | 1.00_27.63 |
| ATOM | 5954 | OG1 THR B 367 | 65.771 -1 | 1.068 | 91.656 | 1.00 28.12 |
| ATOM | 5955 | CG2 THR B 367 | 64.280 -1 | | 89.890 | 1.00 22.94 |
| | | C THR B 367 | 66.197 -1 | | 89.094 | 1.00 25.46 |
| MOTA | 5956 | | | | | |
| MOTA | 5957 | O THR B 367 | 65.389 -1 | | 88.964 | 1.00 24.48 |
| ATOM | 5958 | N LEU B 368 | 66.962 -1 | | 88.092 | 1.00 23.33 |
| ATOM | 5959 | CA LEU B 368 | 66.857 ~1 | 3.990 | 86.785 | 1.00 28.99 |
| | 5960 | CB LEU B 368 | 67.719 -1 | | 85.759 | 1.00 27.67 |
| ATOM | | | | | 85.046 | 1.00.29.47 |
| ATOM · | 5961 | CG LEU B 368 | 67.060 -1 | | | 1 00 22 47 |
| ATOM | 5962 | CD1 LEU B 368 | 65.923 -1 | | 84.195 | 1.00 32.45 |
| ATOM | 5963 | CD2 LEU B 368 | 66.546 <i>-</i> 1 | 1.027 | 86,043 | 1.00 19.43 |
| | | _ | | | • | • |

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Figure 18-91

| MOTA | 596 | 4 C | LE | EU B | 368 | | 67.26 | 2 -15.45 | 4 86.888 | 1 0 | 32.40 |
|--------|------|------|-------|--------------|-----|---|----------------|----------|----------|------|-------|
| ATOM | 596 | 5 0 | I.F | T B | 368 | | | 5 -16.30 | | | |
| ATOM | 596 | | CI. | D | 369 | | | | | | 31.80 |
| | 596 | | \ C1 | 5 | 303 | | | 2 -15.73 | | | 33.59 |
| MOTA | | | M GL | B | 369 | | | 5 -17.10 | | 1.00 | 39.68 |
| ATOM | 596 | | B GI | .U B | 369 | | 69.736 | 5 -17.14 | 1 89.082 | 1.00 | 42.61 |
| ATOM | 596 | 9 C | 3 GL | υв | 369 | | 71.133 | 3 -17.13 | 8 88.537 | | 50.65 |
| ATOM | 597 | 0 CI | O GL | U B | 369 | | 71.469 | -18.44 | 3 87.842 | | 55.81 |
| ATOM | 597: | 1 01 | El GL | JB | 369 | | 72 500 | -18.56 | 1 07.042 | | |
| ATOM | 5972 | | | UB | | | 72.303 | -10.50 | 1 87.299 | 1.00 | 57.42 |
| | | | 22 GL | υ <u>.</u> Β | 202 | | 70.610 | -19.35 | 3 87.841 | | 58.37 |
| MOTA | 5973 | | | UB | | | 67.479 | -17.95 | 4 88.442 | 1.00 | 34.94 |
| ATOM | 5974 | | GL | J B | 369 | | 67.190 | -18.97 | 4 87.827 | | 32.71 |
| ATOM | 5979 | 5 N | LY | S B | 370 | | 66.805 | -17.54 | 1 89.512 | | 34.92 |
| ATOM | 5976 | 5 CA | LY | SB | 370 | | 65,656 | -18.29 | 5 89.993 | 1 00 | 35.12 |
| MOTA | 5977 | 7 CE | I.V | SB | 370 | | | -17.67 | | | |
| ATOM | 5978 | | | SB | | | 02.001 | -17.67 | 9 91.268 | 1.00 | 37.39 |
| | | ** | | | | | 05.879 | -17.91 | 6 92.532 | | 44.70 |
| ATOM | 5979 | | | SB | | | 66.781 | -16.74 | 1 92.892 | 1.00 | 48.10 |
| MOTA | 5980 | | | SB | _ | | 65.956 | -15.53 | 7 93.346 | | 47.82 |
| MOTA | 5981 | . NZ | LYS | 5 B | 370 | | 66.804 | -14.38 | 7 93.786 | | 45.41 |
| ATOM | 5982 | C | LYS | В | 370 | | 64.581 | -18.37 | 5 88.930 | | 33.21 |
| ATOM | 5983 | 0 | | 5 B | | | | -19.40 | | | |
| ATOM | 5984 | | | . B | | | 64 300 | -17.28 | 9 88.773 | 1.00 | 29.52 |
| | 5985 | | | | | | 64.390 | -17.28 | 88.191 | | 31.62 |
| MOTA | | | | B | | - | 63.368 | -17.27 | 4 87.153 | 1.00 | 37.19 |
| ATOM | 5986 | | ببلخ | В | 371 | | | -15.93 | | 1.00 | 35.65 |
| MOTA | 5987 | С | | В | | | 63.572 | -18.431 | 86.181 | 1.00 | 37.79 |
| ATOM | 5988 | 0 | AL | . в : | 371 | | 62.627 | -19.137 | 7 85.838 | 1 00 | 34.46 |
| ATOM | 5989 | N | LYS | В. | 372 | | 64 810 | -18.644 | 85.759 | | 40.10 |
| ATOM | 5990 | CA | | В: | | | 65 147 | -19.698 | 03.733 | | |
| ATOM | 5991 | C | | В | | | 64 746 | -13.030 | | | 40.46 |
| ATOM | 5992 | ŏ | | В. | | | .04.746 | -21.066 | 85.348 | | 43.15 |
| | | | | | _ | | 64.757 | -22:053 | 84.591 | 1.00 | 43.57 |
| MOTA | 5993 | CB | | В | | | 66.654 | -19.694 | 84.517 | 1.00 | 40.51 |
| ATOM | 5994 | CG | | B 3 | | | 67.029 | -18.925 | 83.248 | | 20.00 |
| ATOM | 5995 | CD | LYS | В 3 | 172 | | | -19.390 | | | 20.00 |
| ATOM | 5996 | CE | LYS | B 3 | 72 | | 68.544 | -20.907 | 82.706 | 1 00 | 20.00 |
| ATOM | 5997 | NZ | | B 3 | | | 69 814 | -21:354 | 02.700 | | |
| ATOM | 5998 | N | | B 3 | | | | | | | 20.00 |
| ATOM | 5999 | CA | | B 3 | | | | -21.159 | 86.624 | T.00 | 47.80 |
| | | | | | | | | -22.425 | | | 49.71 |
| ATOM | 6000 | CB | ALA | | 73 | | | -22.639 | | 1.00 | 48.25 |
| ATOM | 6001 | С | ala | | 73 | | 62.515 | -22.443 | 87.494 | 1.00 | 53.38 |
| MOTA | 6002 | 0 | | в 3 | | | 61.844 | -23.313 | 86.903 | 1.00 | 58.01 |
| MOTA | 6003 | OXT | 'Aia | B 3 | 73 | | 62.029 | -21.589 | | 1 00 | 55.13 |
| HETATM | 2991 | ZN | ZN | С | 1 | | 49.660 | 9.211 | | | 32.54 |
| HETATM | | 01 | TSA | | 2 | | 47.669 | | | | |
| HETATM | | 02 | TSA | | 2 | | | 8.189 | | | 28.76 |
| | | | | | | | 49.952 | 6.981 | | | 25.81 |
| HETATM | | 03 | TSA | | 2 | | 52.458 | 5.101 | | 1.00 | 36.93 |
| HETATM | | N1 | TSA | | 2 | | 47.800 | 7.789 | 108.131 | 1.00 | 31.21 |
| HETATM | 2996 | N2 | TSA | D | 2 . | | 53.013 | -1.329 | 101.259 | | 30.57 |
| HETATM | 2997 | C1 | TSA | D | 2 | | 51.859 | 2.799 | 101.610 | | 28.47 |
| HETATM | 2998 | C2 | TSA | D | 2 | | 50.907 | 1.769 | | | 25.57 |
| HETATM | | C3 | TSA | | 2 | | 51.241 | 0.419 | | 1.00 | 23.37 |
| HETATM | | C4 | TSA | | 2 | | | _ | 101:551 | | 21.68 |
| | | | | | | | 52.626 | | 101.366 | | 23.11 |
| HETATM | | C5 | TSA | | 2 | | 53.589 | | 101.303 | 1.00 | 25.02 |
| HETATM | | C6 | TSA | | 2 | | 53.218 | 2.408 | 101.418 | 1.00 | 29.24 |
| HETATM | 3003 | C7 | TSA | D | 2 | | 51.572 | 4.261 | 101.734 | 1.00 | 32.98 |
| HETATM | 3004 | C8 | TSA | D | 2 | | 50.108 | | 101.996 | 1.00 | |
| HETATM | 3005 | C9 | TSA | | 2 | | 50.052 | | 103.338 | | |
| HETATM | 3006 | | TSA | | 2 | | | | | 1.00 | |
| | | | | | 2 | | 49.060 | 5.357 | 104.279 | 1.00 | 25.99 |
| HETATM | | | TSA : | | 2 | | 49.315 | 6.155 | 105.504 | 1.00 | 32.05 |
| HETATM | | | TSA . | | 2 | | 48.515 | 6.184 | 106.595 | 1.00 | 27.37 |
| HETATM | | | TSA : | | 2 | | 48.855 | 6.994 | 107.756 | 1.00 | |
| HETATM | 3010 | C14 | TSA I | D | 2 | | 49.680 | 5.693 | 100.864 | 1.00 | |
| HETATM | 3011 | C15 | TSA I | D | 2 | | 47.776 | 4.545 | 104.132 | 1.00 | |
| HETATM | 3012 | | TSA 1 | | 2 | | 54.438 | | 101.139 | | |
| HETATM | | | TSA I | | 2 | | | -1.703 | | 1.00 | |
| | | | | | | | 52.044 | | 101.316 | 1.00 | |
| HETATM | | ZN | ZN I | Ξ | 1 | | 52.949 | 1.842 | 85.681 | 1.00 | |
| HETATM | | | TSA I | | 2 | | 50.964 | 0.911 | 85.428 | 1.00 | |
| HETATM | 6006 | 02 | TSA I | • | 2 | | 51.255 | 3.324 | 86.654 | 1.00 | |
| | | | | | | | - - | , | | | |

| HETAI | M 600 | 7 03 | TSA | F 2 | 51.569 | 9 6.51 | 2 02 216 | | |
|-----------|--------|-------|--------|------|--------|---------------------|-----------|--------|---------|
| HETAT | M 600 | | | | | | | | 27.89 |
| | M 600 | | | | 50.34 | | | | 27.23 |
| | M 601 | | | | 47.06 | | | | 16.24 |
| | | | _ | | 49.443 | 3 7.57 | 19 93.304 | 1.00 | 27.18 |
| | M 601 | | TSA | F 2 | 48.035 | 7.52 | 9 93.267 | | 25.98 |
| HETAT | M 601 | 2 C3 | TSA | F 2 | 47.227 | | | | 24.59 |
| HETAT | M 601 | 3 C4 | TSA | F 2 | 47.837 | | | 1.00 | 24.33 |
| HETAT | M 601 | | | _ | 49.274 | | | | 25.75 |
| | M 601 | | | _ | | | | , 1.00 | 26.53 |
| | | | TSA | _ | 50.041 | | 9 93.495 | 1.00 | 28.36 |
| | M 601 | | TSA | | 50.349 | 6.40 | 5 93.167 | 1.00 | 25.27 |
| HETAT | M 601 | 7 C8 | TSA | F 2 | 49.716 | | | | 24.18 |
| HETAT | M 6018 | 3 C9 | TSA | | 50.134 | | | 1.00 | |
| HETATI | M 6019 | | | _ | | | | | 27.20 |
| | M 6020 | | 1 TSA | | 49.419 | | | | 30.21 |
| | | | | | 50.118 | | 3 89.327 | 1.00 | 27.18 |
| | M 6021 | | | | 49.762 | 2.62 | 4 88.409 | 1.00 | 23.47 |
| HETATI | M 6022 | C13 | TSA: | F 2 | 50.529 | 2.46 | | 1 00 | 28.28 |
| HETATI | 4 6023 | C14 | TSA . | F 2 | 50.208 | | | 1.00 | 20.20 |
| HETATI | 4 6024 | C15 | TSA | | 48.013 | | | | 28.83 |
| | 4 6025 | | | | | | | | 26.16 |
| | | _ | | | 47.699 | 12.45 | | 1.00 | 27.37 |
| HETAT | | | TSA : | | 45.610 | 11.10 | 7 93.679 | 1.00 | 25.36 |
| HETATA | | | WAT | | 61.391 | 6.72 | 3 88.062 | 1 00 | 12.93 |
| HETATA | 4 6028 | OH2 | WAT (| 3 2 | 55.595 | -4.44 | | | |
| HETATM | 1 6029 | OH2 | WAT (| | 58.656 | | | | 7.53 |
| HETATM | | | WAT | | | | 1 106.749 | | 12.33 |
| | | | | | 46.347 | | 3 111.460 | | 14.54 |
| HETATM | | | WAT | _ | 45.523 | 13.627 | 7 76.224 | 1.00 | 11.14 |
| HETATM | | | WAT | 3 6 | 24.466 | -6.064 | 85.688 | 1.00 | 22.41 |
| HETATM | 6033 | OH2 | WAT (| 3 7 | 48.579 | -17.745 | | 1 00 | 21.99 |
| HETATM | 6034 | OH2 | WAT | 3 8 | | -15.640 | | | |
| HETATM | 6035 | OH2 | | | | | | | 26.67 |
| HETATM | | 022 | | - | 40.554 | -14.901 | | | 23.94 |
| | | Onz | WAT | | 57.540 | -7.620 | 122.771 | 1.00 | 26.96 |
| HETATM | | | WAT G | ; 11 | 59.414 | -2.497 | 84.029 | 1.00 | 22.51 |
| HETATM | 6038 | OH2 | WAT G | 12 | 31.671 | 18.074 | 114.616 | | 32.15 |
| HETATM | 6039 | OH2 | WAT G | 13 | 62.335 | | 117.140 | | |
| HETATM | 6040 | | WAT G | | 45.565 | | | | 19.47 |
| HETATM | | | WAT G | | | 9:469 | | 1.00 | 18.81 |
| HETATM | | | | | 43.311 | 8.237 | | 1.00 | 26.11 |
| | | OH2 | | | 46.628 | 13.883 | 104.423 | 1.00 | 24.28 |
| HETATM | | | WAT G | | 40.672 | 2.507 | 81.576 | 1.00 | 18.30 |
| HETATM | 6044 | OH2 | WAT G | 18 | 61.830 | 10,923 | 77.709 | | 22.27 |
| HETATM | 6045 | OH2 | WAT G | 19 | 57.813 | | 108.580 | | 24.68 |
| HETATM | 6046 | | WAT G | | 48.885 | 5.660 | | | |
| HETATM | | | WAT G | | | | | | 30.00 |
| HETATM | | | | | 36.382 | -8.352 | | | 17.32 |
| | | | WAT G | | | -10.091 | 86.422 | 1.00 | 27.38 |
| HETATM | | | WAT G | 23 | 54.802 | -3.446 | 90.346 | 1.00 | 21.73 |
| HETATM | | OH2 | WAT G | 24 | 49.292 | 12.112 | 140.537 | 1.00 | |
| HETATM | 6051 | OH2 | WAT G | 25 | 56.747 | 8.830 | 60.744 | 1.00 | |
| HETATM | 6052 | OH2 | WAT G | 26 | 41.952 | 9.79 | | 1.00 | 40.67 |
| HETATM | | | WAT G | 27 | | | | 1.00 | |
| HETATM | | | | | 31.268 | | 106.695 | 1.00 | |
| | | | WAT G | 28 | 68.342 | 17.79: | 111.076 | 1.00 | 30.93 |
| HETATM | | | WAT G | 29 | 72.651 | -6.985 | 94.845 | 1.00 2 | 29.34 . |
| HETATM | 6056 | OH2 | WAT G | 30 | 39.287 | 9.257 | 85.623 | 1.00 2 | |
| HETATM | 6057 | OH2 | WAT G | 31 | 61.221 | 14.462 | 87.256 | | |
| HETATM | 6058 | | WAT G | 32 | 38.167 | | 107.435 | | |
| HETATM | | OH2 | WAT G | | | | | 1.00 | |
| | | | | 33 | 64.657 | -2.682 | 96.225 | 1.00 1 | 18.70 |
| HETATM | | | WAT G | 34 | 44.059 | -2.698 ⁻ | 99.805 | 1.00 3 | 30.02 |
| HETATM | 6061 | | WAT G | 35 | 38.480 | 4.763 | 93.051 | 1.00 2 | 28.03 |
| HETATM | 6062 | OH2 : | VAT G | 36 | 57.899 | | 112.976 | 1.00.2 | |
| HETATM | | | VAT G | 37 | 57.092 | | | | |
| HETATM | | | | | | 3.145 | 93.309 | 1.00 2 | |
| | | | VAT G | 38 | 52.194 | | 118.878 | 1.00 3 | 10.83 |
| HETATM | | OH2 V | | 39 | 69.400 | 14.200 | 123.379 | 1.00 3 | 0.98 |
| HETATM (| 5066 | OH2 : | JAT G | 40 | 24.024 | 6.540 | 79.852 | 1.00 3 | |
| HETATM (| 6067 | CH2 ! | | 41 | | 10.880 | 89.402 | | |
| HETATM | | | VAT G | 42 | 24.976 | | | 1.00 2 | |
| HETATM (| | OH2 W | 12 m C | | | | 109.692 | 1.00 4 | |
| | | | | 43 | 46.533 | -4.511 | 94.759 | 1.00 2 | |
| HETATM 6 | | | AT, G | 44 | | 13.833 | 86.306 | 1.00 2 | 7.08 |
| HETATM (| 071 | OH2 W | AT G | 45 | 70.578 | 4.183 | 105.248 | 1.00 4 | |
| HETATM, 6 | 072 | OH2 W | AT G | 46 | 53.938 | | 116.021 | 1.00 3 | |
| • | | | | | | | | | / |

| HETATM | 6073 | OH2 | WAT | 3 47 | 38.4 | 158 -0 | .443 | 63.035 | 1.00 | 28.35 |
|--|------|------|-------|------|--------|--------|-------|---------|------|-------|
| HETHER. | 6074 | | WAT | | 64.7 | 186 7 | 930 | 107.466 | 1.00 | 34.46 |
| HETATM | 6074 | | _ | | 50.8 | | | 114.809 | | 40.51 |
| HETATM | 6075 | | WAT (| | | | | | | - |
| HETATM | 6076 | OH2 | WAT (| 50 | | 63 -10 | | 68.080 | | 39.11 |
| HETATM | 6077 | OH2 | WAT (| 51 | 71.3 | 28 -14 | .321 | 86.007 | 1.00 | 33.30 |
| HETATM | | | WAT | | 63.2 | | .210 | 79.836 | 1.00 | 35.75 |
| neimin | 6070 | | | • | | 63 -12 | | 94.306 | | 29.57 |
| HETATM | 6079 | | VAT | | | | | | | |
| HETATM | 6080 | OH2 | WAT | 5 54 | 46.0 | | .641 | 76.561 | | 27.97 |
| HETATM | 6081 | OH2 | WAT | 55 | 46.6 | 14 -13 | . 620 | 89.775 | 1.00 | 24.25 |
| HETATM | 6082 | | WAT (| | 76.6 | 00 0 | . 622 | 89.097 | 1.00 | 29.19 |
| UEININ | 6002 | | WAT | | 53.5 | | 439 | 79.089 | 1 00 | 34.05 |
| HETATM | 6083 | | | | | | | | | |
| HETATM | 6084 | | WAT | | 71.3 | | .026 | 83.310 | | 35.02 |
| HETATM | 6085 | OH2 | WAT (| 59 | 28.1 | .88 -9 | .956 | 81.594 | | 33.21 |
| HETATM | | OH2 | WAT | 60 | 53.0 | 84 20 | .992 | 98.483 | 1.00 | 27.64 |
| | | | WAT | | 59.4 | | .630 | 93.423 | 1.00 | 30.30 |
| HETATM | | | | | 26.1 | | . 809 | 95.805 | | 33.04 |
| HETATM | | | WAT | | | | | | | |
| HETATM | 6089 | OH2 | WAT (| 63 | 26.0 | | .121 | 89.620 | | 37.39 |
| HETATM | 6090 | OH2 | WAT C | 64 | 47.1 | .00 -б | .141 | 109.711 | 1.00 | 20.88 |
| HETATM | | | WAT C | | . 23.2 | 73 0 | .731 | 92.275 | 1.00 | 30.38 |
| MEIAIM | 6002 | | | | | 40 -24 | | 72.694 | 1 00 | 37.51 |
| HETATM | 6092 | | | | | | | | | 34.63 |
| HETATM | 6093 | | WAT C | | 33.7 | | | 111.676 | | |
| HETATM | 6094 | OH2 | WAT C | 68 | 52.8 | | | 126.276 | | 47.11 |
| HETATM | | OH2 | WAT C | 69 | 50.2 | 18 16 | .953 | 111.099 | 1.00 | 26.24 |
| HETATM | | | WAT C | | 44.7 | | .844 | 70.857 | 1.00 | 24.95 |
| HETAIM | 6030 | | | | | 17 -18 | | 82.921 | | 29.48 |
| HETATM | 6097 | | WAT | | | | | | | 48.70 |
| HETATM | 6098 | | WAT C | | 76.3 | | | 116.550 | | |
| HETATM | 6099 | OH2 | WAT C | 73 | 30.2 | 14 -8 | .086 | 87.873 | | 46.35 |
| HETATM | | OH2 | WAT C | 74 | 45.3 | 20 12 | .061 | 80.458 | 1.00 | 30.80 |
| HETATM | | | WAT C | | 72.8 | 181 5 | .360 | 86.249 | 1.00 | 29.04 |
| | | | | | | 74 -23 | | 87.252 | 7.00 | 41.96 |
| HETATM | | | WAT C | | | | | | | 26.45 |
| HETATM | 6103 | | WAT C | | 40.6 | | | 100.345 | | |
| HETATM | 6104 | OH2 | WAT G | 78 | 41.6 | 66 -19 | | 70.073 | | 36.27 |
| HETATM | 6105 | OH2 | WAT G | 79 | 46.4 | 08 -6 | .539 | 92.717 | 1.00 | 25.78 |
| HETATM | | | WAT G | | 35.7 | 43 -12 | : 230 | 81.646 | 1.00 | 28.34 |
| | | OH2 | WAT C | | 28.2 | | | 121.961 | 1.00 | 41.15 |
| HETATM | | | | | | | .154 | 71.986 | | 32.34 |
| HETATM | | OH2 | WAT G | | 68.8 | | | | | |
| HETATM | 6109 | OH2 | WAT G | | | 25 -11 | . 128 | 85.150 | | 24.14 |
| HETATM | 6110 | OH2 | WAT G | 84 | 75.3 | 74 -1 | .773 | 92.264 | | 26.12 |
| HETATM | 6111 | OH2 | WAT G | 85 | 46.9 | 57 12 | . 230 | 142.271 | 1.00 | 37.07 |
| HETATM | 6112 | | WAT G | | 63.7 | 89 9 | . 551 | 64.329 | 1.00 | 55.58 |
| | | | | | 60.6 | | .185 | 72.215 | | 58.55 |
| HETATM | 6113 | | WAT G | | | | | 82.064 | | 31.10 |
| HETATM | 6114 | | WAT | | 56.5 | | .505 | | | |
| HETATM | 6115 | OH2 | WAT G | 89 | 26.3 | | . 876 | 92.250 | | 29.70 |
| HETATM | | OH2 | WAT G | 90 | 67.6 | 04 -16 | . 583 | 80.808 | 1.00 | 32.85 |
| HETATM | | | WAT G | | 23.9 | | .899 | 82.068 | 1.00 | 42.95 |
| | | | | | 50.0 | | | 117.380 | 1.00 | 30.05 |
| heti im | | | WAT G | | | - | .492 | 83.952 | | 43.59 |
| HET: IM | 6119 | | WAT G | | 26.7 | | | | | |
| HETA.M | 6120 | OH2 | WAT G | 94 | 42.7 | | | 113.787 | | 40.17 |
| HETATM | 6121 | OH2 | WAT G | 95 | 57.9 | 66 7 | . 989 | 134.170 | 1.00 | 47.82 |
| HETATM | | | WAT G | | 54.4 | | .550 | 119.086 | 1.00 | 36.62 |
| BELWIN | C122 | | WAT G | | 53.0 | | | 101.718 | | 41.62 |
| HETATM | 0173 | Onz | WALG | 21 | | | | 68.207 | | 45.98 |
| HETATM | | | WAT G | | | 86 -23 | .045 | | | |
| HETATM | 6125 | OH2 | WAT G | 99 | 54.8 | 55 -9 | .614 | 121.975 | | 34.57 |
| HETATM | | | WAT G | | 57.4 | .08 -3 | .352 | 57.145 | | 42.14 |
| | | OHS | WAT G | 1.01 | 63.5 | 90 20 | .353 | 123.667 | 1.00 | 33.87 |
| HETATM | 0127 | 0112 | WAT G | 102 | | 29 -23 | | 72.392 | | 30.23 |
| HETATM | 0178 | UHZ | MAI G | 102. | | | | | | 52.01 |
| HETATM | 6129 | OH2 | WAT G | T03 | 62.8 | | .913 | 76.094 | | |
| HETATM | 6130 | OH2 | WAT G | 104 | 34.5 | | .529 | 73.089 | | 36.29 |
| HETATM | 6131 | OH2 | WAT G | 105 | 51.5 | 88 20 | .869 | 67.459 | | 36.85 |
| | | ONS | WAT G | 106 | 28.1 | 60 18 | .020 | 129.379 | 1.00 | 42.87 |
| HETATM | | 0112 | WAT G | 107 | | 82 -11 | | 57.603 | | 43.62 |
| HETATM | | UHZ | WAT | 107 | | | | 93.281 | | 41.95 |
| HETATM | 6134 | | WAT G | | 44.7 | | . 605 | | 1.00 | 35 71 |
| HETATM | | OH2 | WAT G | 109 | | 88 -11 | .900 | 94.019 | T.00 | 35.71 |
| HETATM | 6136 | OH2 | WAT G | 110 | 49.5 | 61 22 | .763 | 100.800 | 1.00 | 35.40 |
| ************************************** | 6127 | | WAT G | | 75.8 | 53 10 | .960 | 124.536 | 1.00 | 56.20 |
| HETATM | 073/ | | | | 54.3 | 53 6 | 930 | 136.095 | 1.00 | 36.40 |
| HETATM | 6138 | UH2 | WAT G | 112 | 34.3 | 0) 5 | . 530 | | 4.00 | |
| | | | | | • | | | | | |

210/263 Figure 18-94

| HETATM 6139 OH2 WAT G 113 | 33.114 1.764 67.443 1.00 37.01 |
|---------------------------|---|
| HETATM 6140 OH2 WAT G 114 | 40 610 |
| HETATM 6141 OH2 WAT G 115 | |
| HETATM 6142 OH2 WAT G 116 | |
| HETATM 6143 OH2 WAT G 117 | 50 000 |
| HETATM 6144 OH2 WAT G 118 | |
| HETATM 6145 OH2 WAT G 119 | 2.00 20.00 |
| HETATM 6146 OH2 WAT G 120 | 39.749 -0.616 132.457 1.00 37.43 |
| HETATM 6147 OH2 WAT G 121 | 44.921 1.089 137.137 1.00 40.80 31.081 7.617 75.105 1.00 40.86 |
| HETATM 6148 OH2 WAT G 121 | |
| HETATM 6149 OH2 WAT G 123 | 35.554 12.017 105.965 1.00 33.58 |
| HETATM 6150 OH2 WAT G 123 | 41.381 -23.534 70.872 1.00 38.10 |
| | 31.999 1.992 73.813 1.00 33.97 |
| HETATM 6151 OH2 WAT G 125 | 55.761 10.285 101.654 1.00 47.66 |
| HETATM 6152 OH2 WAT G 126 | 30.596 12.964 133.642 1.00 37.98 |
| HETATM 6153 OH2 WAT G 127 | 59.611 5.347 136.114 1.00 46.39 |
| HETATM 6154 OH2 WAT G 128 | 24.190 12.220 124.679 1.00 30.77 |
| HETATM 6155 OH2 WAT G 129 | 70.078 4.455 86.283 1.00 36.11 |
| HETATM 6156 OH2 WAT G 130 | 57.882 -4.314 125.597 1.00 41.40 |
| HETATM 6157 OH2 WAT G 131 | 45.838 -20.690 65.884 1.00 35.98 |
| HETATM 6158 OH2 WAT G 132 | 47.574 3.186 79.027 1.00 36 67 |
| HETATM 6159 OH2 WAT G 133 | 46.856 -18.901 62.295 1.00 45.40 |
| HETATM 6160 OH2 WAT G 134 | 40.164 5.047 95.358 1.00 31.38 |
| HETATM 6161 OH2 WAT G 135 | 27.268 -0.405 122.461 1.00 38.16 |
| HETATM 6162 OH2 WAT G 136 | 54.200 -20.155 66.212 1.00 37.55 |
| HETATM 6163 OH2 WAT G 137 | 45.435 -10.534 103.626 1.00 37.96 |
| HETATM 6164 OH2 WAT G 138 | 31.633 25.030 106.499 1.00 43.94 |
| HETATM 6165 OH2 WAT G 139 | 79.029 -7.518 93.606 1.00 40.55 |
| UEMAMM 6166 OUR WAR C 340 | 68.597 20.711 111.685 1.00 33.25 |
| HETATM 6167 OH2 WAT G 141 | |
| HETATM 6168 OH2 WAT G 143 | |
| HETATM 6169 OH2 WAT G 144 | |
| HETATM 6170 OH2 WAT G 145 | |
| HETATM 6171 OH2 WAT G 146 | |
| HETATM 6172 OH2 WAT G 147 | |
| HETATM 6173 OH2 WAT G 148 | |
| HETATM 6174 OH2 WAT G 149 | 34.963 10.688 91.806 1.00 31.12 |
| HETATM 6175 OH2 WAT G 150 | 54.859 -15.085 96.769 1.00 46.65 |
| HETATM 6176 OH2 WAT G 151 | 34.695 2.391 131.273 1.00 39.22 |
| HETATM 6177 OH2 WAT G 151 | 40.348 1.395 61.905 1.00 34.09 |
| HETATM 6178 OH2 WAT G 152 | 66.912 17.666 127.489 1.00 45.19 |
| HETATM 6179 OH2 WAT G 154 | 31.096 19.900 103.232 1.00 43.45 |
| | 28.074 -4.222 70.175 1.00 28.86 |
| | 63.586 -1.894 99.003 1.00 41.15 |
| | 54.145 -22.222 88.415 1.00 40.92 |
| HETATM 6182 OH2 WAT G 157 | 62.443 13.765 89.547 1.00 33.69 |
| HETATM 6183 OH2 WAT G 158 | 58.832 9.798 101.311 1.00 31.00 |
| HETATM 6184 OH2 WAT G 159 | 37.701 -5.528 119.322 1 00 45.00 |
| HETATM 6185 OH2 WAT G 160 | 43.599 13.442 131.274 1 00 38.43 |
| HETATM 6186 OH2 WAT G 161 | 23.540 -1.137 96.111 1 00 51.83 |
| HETATM 6187 OH2 WAT G 162 | 59.915 -4.318 110.873 1.00 41.92 |
| HETATM 6188 OH2 WAT G 163 | 51.265 -8.264 60.546 1.00 31.25. |
| HETATM 6189 OH2 WAT G 164 | 58.109 7.024 98.294 1.00 46.30 |
| HETATM 6190 OH2 WAT G 165 | 46.553 18.195 74.179 1.00 37.53 |
| HETATM 6191 OH2 WAT G 166 | 55.706 -21.025 92.515 1.00 43.91 |
| HETATM 6192 OH2 WAT G 167 | 67.146 -1.958 109.704 1.00 43.13 |
| HETATM 6193 OH2 WAT G 168 | 47.445 -3.047 134.746 1.00 27.99 |
| HETATM 6194 OH2 WAT G 169 | 65.193 5.304 63.562 1.00 36.05 |
| HETATM 6195 OH2 WAT G 170 | 36.176 8.979 102.024 1.00 39.63 |
| HETATM 6196 OH2 WAT G 171 | 70.527 5.797 70.886 1.00 44.69 |
| HETATM 6197 OH2 WAT G 172 | |
| HETATM 6198 OH2 WAT G 173 | |
| HETATM 6199 OH2 WAT G 174 | |
| HETATM 6200 OH2 WAT G 175 | |
| HETATM 6201 OH2 WAT G 175 | |
| | 36.771 -6.815 121.530 1.00 32.57 |
| HETATM 6202 OH2 WAT G 177 | 63.224 7.776 89.317 1.00 29.83 |
| HETATM 6203 OH2 WAT G 178 | 29.606 15.345 132.470 1.00 47.28 |
| ETATM 6204 OH2 WAT G 179 | 52.811 11.799 98.957 1.00 36.09 |

| HETATM | 6205 | OH2 | WAT G | 180 | 38.589 | 18.249 | 88.356 | 1.00 36.19 |
|---------|------|-----|-------|-----|----------------------------|------------------------------|---------|------------|
| HETATM | 6206 | OH2 | WAT G | 181 | 43.734 | -15.681 | 61.135 | 1.00 34.24 |
| HETATM | 6207 | | WAT G | | 42.283 | 15.251 | 91.437 | 1.00 37.96 |
| HETATM | | | WAT G | | | -11.129 | 126.206 | 1.00 45.78 |
| HETATM | 6209 | OH2 | | | 50.011 | -19.367 | 92.127 | 1.00 36.55 |
| HETATM | | | WAT G | | 56.880 | | | 1.00 39.12 |
| | | | WAT G | | 26.356 | | 125.052 | 1.00 32.68 |
| HETATM | | | | | | | | |
| HETATM | | | WAT G | | 24.631 | | 122.650 | 1.00 45.67 |
| HETATM | | | WAT G | | 23.516 | 4.964 | 81.599 | 1.00 42.16 |
| HETATM | 6214 | | WAT G | | 55.017 | 14.964 | 62.948 | 1.00 50.18 |
| HETATM | 6215 | | WAT G | | 33.371 | | 105.640 | 1.00 37.04 |
| HETATM | 6216 | OH2 | WAT G | 191 | .44.466 | -10.386 | 91.144 | 1.00 36.62 |
| HETATM | 6217 | OH2 | WAT G | 192 | 28.437 | 22.668 | 121.285 | 1.00 38.19 |
| HETATM | 6218 | OH2 | WAT G | 193 | 29.786 | 24.957 | 122.112 | 1.00 42.05 |
| HETATM | | OH2 | WAT G | 194 | 28.852 | 3.461 | 96.101 | 1.00 48.35 |
| HETATM | | OH2 | WAT G | 195 | 28.852 41.681 26.812 | 11.318 | 92.011 | 1.00 32.60 |
| HETATM | | | WAT G | | 26.812 | -10.229 | 111.631 | 1.00 47.70 |
| HETATM | | | WAT G | | 42.432 | -10.229 -23.250 12.756 | 76.629 | 1.00 48.86 |
| HETATM | | | WAT G | | 25.484 | 12.756 | 121.410 | 1.00 43.09 |
| HETATM | | | WAT G | | | -20.514 | | 1.00 46.80 |
| | | OH2 | | | | -13.079 | | 1.00 44.89 |
| HETATM | | OH2 | | | 59.982 | | 103.984 | 1.00 40.63 |
| HETATM | | | | | 67 164 | -12.771 | | 1.00 35.13 |
| HETATM | | | WAT G | | | | 79.238 | 1.00 33.13 |
| HETATM | | | WAT G | | 28.708 | 9.211 | | |
| HETATM | | | WAT G | | 53.256 | | 122.243 | 1.00 48.49 |
| HETATM | | | WAT G | | 50.706 | 16.208 | 87.357 | 1.00 41.26 |
| HETATM | | | WAT G | | 50.000 | 34.998 | | 1.00 39.15 |
| HETATM | | OH2 | | | | -16.236 | | 1.00 29.70 |
| HETATM | 6233 | | WAT G | | 24.395 | | 111.635 | 1.00 50.82 |
| HETATM | 6234 | | WAT G | | 53.384 | | 114.289 | 1.00 44.49 |
| HETATM | 6235 | | WAT G | | 60.120 | -9.482 | 94.788 | 1.00 31.97 |
| HETATM | 6236 | OH2 | WAT G | 211 | 23.405 | | 111.744 | 1.00 44.97 |
| HETATM | | OH2 | WAT G | 212 | 46.214 | 20.943 | 76.878 | 1.00 59.14 |
| HETATM | | OH2 | WAT G | 213 | 29.754 | 6:983 | 97.109 | 1.00 41.78 |
| HETATM | 6239 | OH2 | WAT G | 214 | 46.820 | -0.465 | 55.181 | 1.00 41.02 |
| HETATM | | OH2 | WAT G | 215 | 59.143 | 22.096 | 124.775 | 1.00 38.42 |
| HETATM | 6241 | OH2 | WAT G | 216 | 42.674 | 14.088 | 66.037 | 1.00 32.50 |
| HETATM | | OH2 | WAT G | 217 | 55.009 | -7.248 | 98.186 | 1.00 56.50 |
| HETATM | | OH2 | WAT G | 218 | 63.361 | -8.209 | 109.653 | 1.00 49.66 |
| HETATM | | OH2 | WAT G | 219 | 66.583 | -8.146 | 94.671 | 1.00 50.91 |
| HETATM | 6245 | | WAT G | | | 2.583 | 93.919 | 1.00 36.99 |
| HETATM | 6246 | | WAT G | | 24.470 | -8.606 | 79.502 | 1.00 47.24 |
| HETATM | | | WAT G | | 76.913 | -7.777 | 83.973 | 1.00 50.43 |
| HETATM | | | WAT G | | 32.788 | | 129.136 | 1.00 42.47 |
| HETATM | | | WAT G | | | -16.880 | | 1.00 46.69 |
| HETATM | | | WAT G | | 78.567 | -2.802 | 93.970 | 1.00 43.17 |
| HETATM | 6251 | | WAT G | | 45.681 | 1.248 | | 1.00 35.84 |
| HETATM | 6252 | | WAT G | | 38.263 | 15.236 | | 1.00 42.39 |
| HETATM | 6252 | | WAT G | | 38.933 | 35 224 | 108.488 | 1.00 52.23 |
| HETATH | 6253 | | WAT G | | 33.755 | 14.939 | | 1.00 46.56 |
| HETATM | 6254 | | WAT G | | | | 100.859 | |
| HETATM | 6255 | | | | 34.140 | | 63.039 | 1.00 31.02 |
| HETATM | 6256 | | WAT G | | 34.140 | 0.565 | 81.662 | 1.00 39.83 |
| HETATM | 6257 | | WAT G | | 37.277 | 13.977 | 93.216 | |
| HETATM' | 6258 | | WAT G | | 57.307 | 5.947 | | 1.00 28.55 |
| HETATM | 6259 | | WAT G | | 31.718 | 16.820 | 125.707 | 1.00 53.16 |
| HETATM | 6260 | | WAT G | | 60.624 | 31.119 | 110.067 | 1.00 51.02 |
| HETATM | 6261 | | WAT G | | 44.357 | 4.267 | 94.916 | 1.00 57.50 |
| HETATM | 6262 | | WAT G | | 68.454 | 1.072 | 70.111 | 1.00 38.65 |
| HETATM | 6263 | OH2 | WAT G | 238 | 27.836 | 6.773 | 79.253 | 1.00 44.95 |
| HETATM | 6264 | OH2 | WAT G | 239 | . 54.933 | 23.344 | 81.087 | 1.00 42.95 |
| HETATM | 6265 | OH2 | WAT G | 240 | 34.072 | -15.271 | 71.579 | 1.00 45.78 |
| HETATM | 6266 | OH2 | WAT G | 241 | 35.966 | -1.059 | 61.973 | 1.00 38.91 |
| HETATM | 6267 | | WAT G | | 29.687 | 1.898 | 127.376 | 1.00 44.85 |
| HETATM | 6268 | | WAT G | | | -10.150 | 113.501 | 1.00 38.32 |
| HETATM | 6269 | | WAT G | | 57.252 | 9.773 | 96.696 | 1.00 48.83 |
| HETATM | 6270 | | WAT G | | 62.310 | 13.262 | 80.972 | 1.00 38.54 |
| HEIVIN | 02,0 | | | ~ | | | | |

| HETAT. | M 6271 | OH2 WAT G 246 | | 50.24 | 8 ~5.552 | 2 102.815 | 1.00 43.23 |
|------------------|--------|---------------------------------|---|------------------|-------------------|-------------------|--------------------------|
| HETAT | M 6272 | OH2 WAT G 247 | | 47.96 | | | |
| HETAT | M 6273 | OH2 WAT G 248 | | 62.50 | | 6 108.414 | |
| HETAT | | | | 53.97 | 1 19.763 | 3 61.067 | |
| HETAT | M 6275 | | | 38.40 | 9.828 | | |
| HETATI | | | | 35.304 | 4 -6.179 | 66.319 | |
| HETATI | | | | 39.218 | 3 -12.667 | | 1.00 36.17 |
| HETATI | | | • | 56.35 | | | 1.00 46.38 |
| HETATI | | | | 69.850 | | 5 122.119 | 1.00 55.07 |
| HETATI | | _ | | 75.703 | | | 1.00 30.64 |
| HETATI | | | - | | | 113.965 | 1.00 34.48 |
| HETATI HETATI | | | | 54.081 | | | 1.00 39.11 |
| HETATI | | | | 32.801 45.040 | | | 1.00 35.72 |
| HETATA | | | | 39.815 | | 128.855 | 1.00 36.57 1.00 40.10 |
| HETATY | | | | 28.763 | | | 1.00 44.39 |
| HETATN | | OH2 WAT G 262 | | | | 60.539 | 1.00 50.89 |
| HETATI | | OH2 WAT G 263 | | 64.353 | | 117.495 | 1.00 62.67 |
| HETATM | | OH2 WAT G 264 | | | | 128.124 | 1.00 50.42 |
| HETATM | 6290 | OH2 WAT G 265 | | 75.183 46.289 | 6.826 | 52.485 | 1.00 46.86 |
| HETATM | | OH2 WAT G 266 | | 68.708 | 13.973 | 70.958 | 1.00 37.90 |
| HETATM | | OH2 WAT G 267 | | 71.504 | | 130.029 | 1.00 38.78 |
| HETATM | | OH2 WAT G 268 | | 36.309 | | 130.364 | 1.00 42.92 |
| HETATM | | OH2 WAT G 269 OH2 WAT G 270 | | 65.973 | | | 1.00 51.68 |
| HETATM | | OH2 WAT G 270 OH2 WAT G 271. | | 71.952 | 13.021 ~17.578 | | 1.00 37.70 |
| HETATM | | OH2 WAT G 271. | | 26.917 | | | 1.00 49.33 1.00 38.07 |
| HETATM | | OH2 WAT G 273 | | 63.380 | | 126.550 | |
| HETATM | | OH2 .WAT G 274 | | 63.360 | | | 1.00 37.54 |
| HETATM | 6300 | OH2 WAT G 275 | | | -13.015 | | 1.00 37.42 |
| HETATM | 6301 | OH2 WAT G 276 | | 26.406 | 25.831 | 117.328 | 1.00 48.37 |
| HETATM | | OH2 WAT G 277 | | | -10.251 | 98.201 | 1.00 46.36 |
| HETATM | | OH2 WAT G 278 | | 30.343 | | 117.764 | 1.00 49.87 |
| HETATM | | OH2 WAT G 279 . | | 45.135 | | 111.056 | 1.00 43.93 |
| HETATM HETATM | | OH2 WAT G 280 OH2 WAT G 281 | | 50.553 | | 120.511 | 1.00 54.02 |
| HETATM | | OH2 WAT G 281 | | 60.428 30.342 | 13.652 2.204 | | 1.00 31.10 |
| HETATM | | OH2 WAT G 283 | | 60.358 | | 127.736 | 1.00 45.19 1.00 33.17 |
| HETATM | | OH2 WAT G 284 | | 64.193 | 3.421 | 62.117 | 1.00 45.81 |
| HETATM | | OH2 WAT G 285 | | 45.468 | 6.113 | | 1.00 48.98 |
| HETATM | 6311 | OH2 WAT G 286 | | 47.514 | 3.808 | 98.279 | 1.00 46.45 |
| HETATM | | OH2 WAT G 287 | | 72.144 | -6.345 | 77.930 | 1.00 40.04 |
| HETATM | | OH2 WAT G 288 | | 54.142 | -5.100 | 99.674 | 1.00 43.62 |
| HETATM | | OH2 WAT G 289 | | 48.982 | 13.297 | 65.822 | 1.00 46.98 |
| HETATM | | OH2 WAT G 290 | | 41.171 | 34.107 | | 1.00 51.76 |
| HETATM HETATM | | OH2 WAT G 291 OH2 WAT G 292 | | 36.494 48.580 | 37.195 23.117 | 104.170 85.456 | 1.00 44.27 1.00 40.96 |
| HETATM | | OH2 WAT G 293 | | 55.853 | 22.934 | 98.099 | 1.00 40.95 |
| HETATM | | OH2 WAT G 294 | | 61.720 | 11.077 | 89.427 | 1.00 41.21 |
| HETATM | | OH2 WAT G 295 | | | -18.552 | | 1.00 42.32 |
| HETATM | 6321 | OH2 WAT G 296 | | | | | 1.00 37.41 |
| HETATM | 6322 | OH2 WAT G 297 | | 70.258 | 24.928 | 82.843 | 1.00 48.09 |
| HETATM | 6323 | OH2 WAT G 298 | | 77.493 | 0.940 | 130.507 | 1.00 51.77 |
| HETATM | 6324 | OH2 WAT G 299 | | 32.233 | 12.182 | 83.028 | 1.00 53.51 |
| HETATM | | OH2 WAT G 300 | | 40666 | 12.878 | 65.747 | 1.00 46.49 |
| HETATM | | OH2 WAT G 301 | | 50.977 | 12.831 | 114.597 | 1.00 48.51 |
| HETATM | | OH2 WAT G 302 | | 54.236 | 3.817 | 92.196 | 1.00 41.15 |
| HETATM HETATM | | OH2 WAT G 303 OH2 WAT G 304 | | 59.527 | -1.343 | 107.471 | 1.00 36.71 |
| HETATM | | CH2 WAT G 305 | | 70.331 | 3.940 6.969 | 89.312 127.780 | 1.00 47.70 1.00 41.96 |
| HETATM | | OH2 WAT G 306 | | 42.156 | -0.139 | 133.156 | 1.00 41.98 |
| HETATM | | OH2 WAT G 307 | | 58.886 | 16.514 | 99.413 | 1.00 53.60 |
| HETATM | | OH2 WAT G 308 | | 67.617 | -1.589 | 96,570 | 1.00 40.36 |
| HETATM | | OH2 WAT G 309 | | | -10.936 | 98.849 | 1.00 48.80 |
| HETATM | | OH2 WAT G 310 | | 45.576 | 25.388 | 131.914 | 1.00 48.99 |
| MTATE | 6336 | CH2 WAT G 311 | | 37.583 | -6.243 | 64.257 | 1.00 37.06 |
| • | | | | | | • | |

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Figure 18-97

| HETATN | 4 6337 | OH2 | 6ta m | G 312 | | 66.759 | 16.408 | 94.600 | 1.00 45.07 | , |
|------------------|--------|-------|----------------------------------|---------|---|--------|---------|---------|------------|-----|
| | | | | | | | | | | |
| HETATA | | | | G 313 | | 24.142 | | 113.340 | 1.00 52.23 | |
| HETATM | | | | G 314 | | 69.409 | | 64.230 | 1.00 39.88 | |
| HETATM | | | | G 315 | | 22.064 | | 115.328 | 1.00 50.23 | |
| HETATM | 6341 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | G 316 | | 50.171 | 9.551 | 100.345 | 1.00 37.32 | : |
| HETATM | 6342 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | G 317 | | 55.104 | 31.302 | 119.497 | 1.00 44.78 | ì |
| HETATM | 6343 | OH2 | WAT | G 318 | | 65.333 | -10.105 | 95.866 | 1.00 44.21 | |
| HETATM | | | | G 319 | | 31.415 | | 128.127 | 1.00 41.95 | _ |
| HETATM | - | | | G 320 | | 37.423 | 13.143 | 88.069 | 1.00 44.79 | |
| | | | | | | | | | | |
| HETATM | | | | G 321 | | 43.619 | 14.292 | 96.509 | 1.00 54.69 | |
| HETATM | | | | G 322 | | 68.048 | | 126.016 | 1.00 42.75 | |
| HETATM | | | | G 323 | | 34.778 | | 130.204 | 1.00 37.06 | j . |
| HETATM | | OH2 | WAT | G 324 | • | 27.972 | 18.144 | 103.841 | 1.00 47.34 | Į |
| HETATM | 6350 | OH2 | WAT | G 325 | | 53.550 | 23.610 | 97.592 | 1.00 38.03 | į |
| HETATM | | OH2 | WAT | G 326 | | 33.776 | 4.171 | 103.451 | 1.00 50.60 | į |
| HETATM | 6352 | | | G 327 | | 37.862 | | 114.870 | 1.00 48.34 | |
| HETATM | | | | G 328 | | 50.893 | 14.612 | 93.478 | 1.00 38.77 | |
| | | | | G 329 | | | -20.913 | 86.137 | | |
| HETATM | | | | | | | | | 1.00 47.69 | |
| HETATM | | | | G 330 | | 50.310 | -23.133 | 74.502 | 1.00 41.94 | |
| HETATM | | | | G 331 | | 41.520 | 7.269 | 60.583 | 1.00 54.93 | |
| HETATM | | | WAT | | | 75.879 | | 106.089 | 1.00 44.65 | 1 |
| HETATM | 6358 | OH2 | WAT | G 333 | | 51.923 | 9.027 | 138.493 | 1.00 41.08 | ; |
| HETATM | 6359 | OH2 | WAT (| 334 | | 49.511 | 27.611 | 79.363 | 1.00 39.05 | ı |
| HETATM | | OH2 | WAT (| G 335 | | 69.385 | 0.852 | 110.192 | 1.00 41.42 | |
| HETATM | | | WAT (| | | 40.952 | 2.479 | | 1.00 42.50 | |
| HETATM | | | WAT | | | 32.998 | | 103.784 | 1.00 54.22 | |
| HETATM | 6363 | | WAT | | | 54.366 | | 136.205 | 1.00 52.69 | |
| | | | | | | | | | | |
| HETATM | | | WAT | | | 35.674 | 13.727 | 89.792 | 1.00 35.83 | |
| HETATM | | | WAT (| | | | -21.361 | 87.138 | 1.00 46.26 | |
| HETATM | | | WAT (| | | 72.053 | | 131.550 | 1.00 45.27 | |
| HETATM | | OH2 | WAT C | 342 | | 28.072 | -1.358 | 70.419 | 1.00 34.92 | |
| HETATM | 6368 | OH2 | WAT (| 3 3 4 3 | | 23.611 | -3.981 | 76.422 | 1.00 52.39 | |
| HETATM | 6369 | OH2 | WAT (| 344 | | 53.684 | 2.564 | 122.150 | 1.00 58.16 | |
| HETATM | | OH2 | WAT C | 345 | | 30.624 | -6:528 | 125.556 | 1.00 34.71 | |
| HETATM | 6371 | | WAT C | | | 27.870 | | 113.997 | 1.00 44.91 | |
| HETATM | | | WAT C | | | 31.903 | -9.588 | | 1.00 55.34 | |
| HETATM | | | WAT C | | | 71.763 | 15.094 | 63.739 | 1.00 48.99 | |
| | | | WAT | | | 25.258 | | 114.760 | 1.00 37.19 | |
| HETATM | C375 | | | | | | | | | |
| HETATM | 63/5 | | WAT G | | | 43.765 | 12.162 | 78.143 | 1.00 42.32 | |
| HETATM | 6376 | | WAT C | | | 32.452 | 5.338 | 73.909 | 1.00 33.70 | |
| HETATM | | | WAT G | | | 52.896 | ~5.770 | | 1.00 46.40 | |
| HETATM | 6378 | OH2 | WAT G | 353 | • | 47.968 | | 115.852 | 1.00 34.62 | |
| HETATM | 6379 | OH2 | WAT G | 354 | | 38.561 | -9.302 | 90.596 | 1.00 49.80 | |
| HETATM | 6380 | OH2 | WAT G | 355 | (| 63.791 | 17.454 | 74.354 | 1.00 56.40 | |
| HETATM | 6381 | OH2 | WAT G | 356 | | 41.360 | 2.648 | 133.760 | 1.00 50.00 | |
| HETATM | 6382 | | WAT G | _ | | 12.467 | | 122.328 | 1.00 38.01 | |
| HETATM | 6383 | | WAT G | | | 50.890 | | 116.668 | 1.00 39.26 | |
| | | | WAT G | | | | -23.881 | 67.865 | 1.00 55.18 | |
| HETATM HETATM | 6305 | | WAT G | | | | | 105.032 | 1.00 38.83 | |
| HETATM | 6365 | | | | | 4.959 | | | | |
| HETATM | 0286 | | WAT G | | | | -19.846 | 82.288 | 1.00 38.60 | |
| HETATM | 6387 | | WAT G | | | 12.245 | -1.140 | 93.572 | 1.00 31.47 | |
| HETATM | 6388 | OH2 I | WAT G | 363 | 7 | 73.552 | 17.770 | 125.885 | 1.00 54.89 | |
| HETATM | 6389 | OH2 | WAT G | 364 | • | 8.769 | 15.898 | 106.810 | 1.00 45.53 | |
| HETATM | 6390 | OH2 V | NAT G | 365 | 3 | 7.543 | 19.031 | 78.866 | 1.00 45.15 | |
| HETATM | 6391 | | WAT G | | | 55.583 | 6.906 | 95.087 | 1.00 44.99 | |
| HETATM | 6392 | | VAT G | | | 1.284 | 9.699 | 78.250 | 1.00 36.58 | • |
| HETATM | 6303 | | NAT G | | | 5.203 | 5.332 | 126.362 | 1.00 46.60 | |
| upinin | 2201 | | | | | | | 95.104 | 1.00 47.85 | |
| HETATM | 6300 | | VAT G | | | 4.742 | ~5.006 | | | |
| HETATM | C250 | OH2 V | | | | 0.349 | 19.871 | 69.925 | 1.00 51.46 | |
| HETATM | 6396 | OH2 | | | | 2.936 | 20.631 | 94.720 | 1.00 38.66 | |
| HETATM | 6397 | OH2 V | | | | | -16.114 | 114.141 | 1.00 44.01 | |
| HETATM | 6398 | OH2 | VAT G | 373 | 3 | 3.863 | 16.838 | 100.275 | 1.00 44.66 | |
| HETATM | 6399 | OH2 W | VAT G | 374 | 2 | 1.613 | 12.569 | 86.140 | 1.00 43.89 | |
| HETATM | 6400 | OH2 W | VAT G | | | | | 100.583 | 1.00 53:53 | |
| HETATM | 6401 | OH2 W | | | _ | 0.095 | 13.395 | 117.505 | 1.00 52.02 | |
| HETATM | 6402 | OH2 | | | | 1.853 | 19.108 | | 1.00 46.47 | |
| BETWIN | | | | | - | | | • | | |
| | | | | | | | | | | |

| HETATM 6403 OH2 WAT G 378 | FF FF |
|----------------------------|---|
| | 55.780 -14.986 65.487 1.00 49.09 |
| HETATM 6404 OH2 WAT G 379 | 40.990 21.205 91.611 1.00 41.02 |
| HETATM 6405 OH2 WAT G 380 | 48.157 1.057 116.992 1.00 44.84 |
| HETATM 6406 OH2 WAT G 381 | |
| | |
| | 30.221 27.743 109.194 1.00 39.92 |
| HETATM 6408 OH2 WAT G 383 | 49.926 -12.826 118.421 1.00 58.95 |
| HETATM 6409 OH2 WAT G 384 | 42.435 -17.636 81.477 1.00 48.47 |
| HETATM 6410 OH2 WAT G 385 | |
| , | 58.226 -25.990 71.378 1.00 48.18 |
| HETATM 6411 OH2 WAT G 386 | 40.495 17.944 128.741 1.00 43.82 |
| HETATM 6412 OH2 WAT G 387 | 31.943 6.301 109.475 1.00 35.53 |
| HETATM 6413 OH2 WAT G 388 | 47.277 2.559 100.509 1.00 43.00 |
| HETATM 6414 OH2 WAT G 389 | |
| | 38.862 9.112 102.620 1.00 31.70 |
| HETATM 6415 OH2 WAT G 390. | 71.652 14.568 105.167 1.00 49.63 |
| HETATM 6416 OH2 WAT G 391 | 68.554 -10.518 73.331 1.00 38.16 |
| | |
| | 70.496 -16.160 84.425 1.00 32.16 |
| HETATM 6418 OH2 WAT G 393 | |
| HETATM 6419 OH2 WAT G 394 | 56.172 15.369 55.027 1.00 47.44 |
| HETATM 6420 OH2 WAT G 395 | 46.150 -9.441 99.999 1.00 47.98 26.892 -8.356 89.057 1.00 34.99 |
| HETATM 6421 OH2 WAT G 396 | 26 002 0 356 00 057 1 00 31.90 |
| | 26.892 -8.356 89.057 1.00 34.99 |
| HETATM 6422 OH2 WAT G 397 | 31.737 14.380 90.395 1.00 50.78 36.261 -13.824 62.777 1.00 50.86 |
| HETATM 6423 OH2 WAT G 398 | 36.261 -13.824 62.777 1.00 50.86 |
| HETATM 6424 OH2 WAT G 399 | 37.312 15.242 134.977 1.00 43.57 |
| HETATM 6425 OH2 WAT G 400 | |
| | 33.728 13.773 126.419 1.00 57.13 |
| HETATM 6426 OH2 WAT G 401 | 45.269 27.937 130.311 1.00 49.55 |
| HEIRIM 0427 ORZ WAI G 402 | 44.887 -17.414 111.508 1.00 54.29 |
| HETATM 6428 OH2 WAT G 403 | 68.928 0.455 136.711 1.00 49.90 |
| HETATM 6429 OH2 WAT G 404 | 43 073 03 573 64 405 1 50 49.90 |
| | 43.271 -21.571 64.425 1.00 48.61 |
| HETATM 6430 OH2 WAT G 405 | 24.243 -4.781 108.590 1.00 51.05 |
| HETATM 6431 OH2 WAT G 406 | 54.828 5.311 59.009 1.00 43.43 |
| HETATM 6432 OH2 WAT G 407 | 53.460 27.992 124.076 1.00 47.83 |
| HETATM 6433 OH2 WAT G 408 | |
| | |
| HETATM 6434 OH2 WAT G 409 | 71.497 15.287 113.071 1.00 34.52 |
| HETATM 6435 OH2 WAT G 410 | 36.407 -18.480 110.466 1.00 55.43 |
| HETATM 6436 OH2 WAT G 411 | 26.220 -9.551 78.158 1.00 47.69 |
| HETATM 6437 OH2 WAT G 412 | |
| | |
| HETATM 6438 OH2 WAT G 413 | 76.173 14.097 122.253 1.00 44.90 |
| HETATM 6439 OH2 WAT G 414 | 58.379 6.335 123:024 1.00 54.61 |
| HETATM 6440 OH2 WAT G 415 | 72.162 -16.705 82.719 1.00 50.63 |
| HETATM 6441 OH2 WAT G 416 | 63.557 26.152 65.944 1.00 39.83 |
| HETATM 6442 OH2 WAT G 417 | 20.007 20.102 00.944 1.00 39.85 |
| | 38.935 23.070 122.742 1.00 52.57 |
| HETATM 6443 OH2 WAT G 418 | 55.256 -10.714 124.501 1.00 42.38 |
| HETATM 6444 OH2 WAT G 419 | 55.443 -9.037 110.170 1.00 46.47 |
| HETATM 6445 OH2 WAT G 420 | 73.873 16.578 123.288 1.00 46.54 |
| HETATM 6446 OH2 WAT G 421 | |
| | 74.426 12.663 117.527 1.00 43.62 |
| HETATM 6447 OH2 WAT G 422 | 52.374 -0.368 51.502 1.00 56.99 |
| HETATM 6448 OH2 WAT G 423 | 60.339 20.215 84.713 1.00 36.27 |
| HETATM 6449 OH2 WAT G 424 | 48.308 1.354 54.561 1.00 38.53 |
| HETATM 6450 OH2 WAT G 425 | |
| | |
| HETATM 6451 OH2 WAT G 426 | 33.222 -14.916 119.528 1.00 51.12 |
| HETATM 6452 OH2 WAT G 427 | 47.477 3.359 112.298 1.00 46.10 |
| HETATM 6453 OH2 WAT G 428 | 39.909 2.272 138.388 1.00 35.33 |
| | 59.309 2.272 136.366 1.00 35.33 |
| · - · · - • • • • • • | 57.829 15.336 126.262 1.00 62.59 |
| HETATM 6455 OH2 WAT G 430 | 48.917 -5.857 119.191 1.00 51.45 |
| HETATM 6456 OH2 WAT G 431 | 44.139 -3.812 132.964 1.00 44.91 |
| HETATM 6457 OH2 WAT G 432 | 38.885 18.594 95.398 1.00 50.23 |
| | |
| HETATM 6458 OH2 WAT G 433 | 52.628 -7.064 55.271 1.00 39.96 |
| HETATM 6459 OH2 WAT G 434 | 60.644 -0.731 101.129 1.00 47.30 |
| HETATM 6460 OH2 WAT G 435 | 64.772 5.808 71.942 1.00 50.81 |
| HETATM 6461 OH2 WAT G 436 | 39.571 16.705 80.180 1.00 34.07 |
| | |
| HETATM 6462 OH2 WAT G 437 | 32.791 -0.551 65.371 1.00 41.40 |
| HETATM 6463 OH2 WAT G 438 | 58.318 -7.989 60.087 1.00 46.94 |
| HETATM 6464 OH2 WAT G 439 | 26.982 5.474 120.408 1.00 46.28 |
| HETATM 6465 OH2 WAT G 440 | |
| | |
| HETATM 6466 OH2 WAT G 441 | 29.494 10.971 118.393 1.00 56.30 |
| HETATM 6467 OH2 WAT G 442 | 69.232 5.594 113.941 1.00 58.17 |
| HETATM 6468 OH2 WAT G 443 | 61.459 11.576 71.140 1.00 61.67 |
| | |

| HETATM | 6469 | он2 | WAT | G | 444 | 59.592 | 2.195 | 58.518 | 1.00 | 42.66 |
|--------|------|-----|------|---|-----|--------|---------|---------|------|-------|
| HETATM | 6470 | OH2 | _WAT | G | 445 | 47.407 | 6.152 | 111.310 | 1.00 | 45.14 |
| HETATM | 6471 | OH2 | WAT | G | 446 | 36.254 | 18.203 | 99.930 | 1.00 | 44.76 |
| HETATM | 6472 | OH2 | TAW | G | 447 | 49.525 | 32.050 | 116.235 | 1.00 | 47.72 |
| HETATM | 6473 | OH2 | TAW | G | 448 | 21.801 | -5.358 | 81.109 | 1.00 | 42.07 |
| HETATM | 6474 | OH2 | WAT | G | 449 | 52.131 | -14.007 | 95.380 | 1.00 | 40.76 |
| HETATM | 6475 | OH2 | TAW | G | 450 | 39.712 | -19.983 | 72.499 | 1.00 | 51.69 |
| HETATM | 6476 | OH2 | WAT | G | 451 | 67.651 | 5.620 | 67.102 | 1.00 | 42.38 |
| HETATM | 6477 | OH2 | WAT | G | 452 | 77.344 | 1.313 | 79.207 | 1.00 | 63.64 |
| HETATM | 6478 | OH2 | WAT | G | 453 | 55.249 | -29.426 | 86.187 | 1.00 | 44.98 |
| HETATM | 6479 | OH2 | WAT | G | 454 | 64.429 | -11.004 | 98.104 | 1.00 | 49.12 |
| HETATM | 6480 | он2 | WAT | G | 455 | 45.456 | -0.814 | 129.510 | 1.00 | 61.60 |
| HETATM | 6481 | OH2 | WAT | G | 456 | 65.066 | -14.790 | 68.028 | 1.00 | 40.08 |
| HETATM | 6482 | OH2 | WAT | G | 457 | 34.732 | 5.611 | 94.924 | 1.00 | 58.32 |

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Figure 19-1

| | Residu | e il X | Y | 7 | ъ о | |
|------|-----------------|------------------|------------------|------------------|--------------------------|--------------|
| atom | 1 CE ALA A 2 | 45.86 | | Z 9 75.022 | B Segment | |
| ATOM | 2 C ALA A 2 | 46.76 | | | | AAAA |
| ATOM | 3 0 ALA A 2 | 46.33 | | | | AAAA |
| ATOM | 4 11 ALA A 2 | 48.28 | | | | AAAA |
| ATOM | 5 CA ALA A 2 | 47.06 | | | | AAAA |
| ATOM | 6 N LYS A 3 | 46.97 | | | | AAAA |
| ATCM | 7 CA LYS A 3 | 46.72 | | | | አጸጸአ |
| ATOM | 8 CE LYS A 3 | 47.81 | | | | AAAA |
| MOTA | 9 CG LYS A 3 | 49.223 | | | | AAAA |
| ATOM | 10 CD LYS A 3 | 50.252 | | | | AAAA |
| ATOM | 11 CE LYS A 3 | 51.654 | | | | AAAA |
| ATOM | 12 NZ LYS A 3 | 52.643 | | | | AAAA |
| ATOM | 13 C LYS A 3 | 45.393 | | | | AAAA |
| ATOM | 14 0 LYS A 3 | 44.894 | | _ | | AAAA |
| ATOM | 15 N VAL A 4 | | | | 1.00 49.33 | AAAA |
| ATOM | 16 CA VALA 4 | 44.826 | _ | | 1.00 46.23 | AAAA |
| ATOM | 17 CB VAL A 4 | 43.561 | | | 1.00 42.51 | AAAA |
| ATOM | 18 CG1 VAL A 4 | 42.543 | | | 1.00 42.26 | AAAA |
| ATOM | 19 CG2 VAL A 4 | 41.213 | | | 1.00 41.51 | aaaa |
| ATOM | 20 C VALA 4 | 42.401 | | | 1.00 42.00 | AAAA |
| ATOM | 21 0 VALA 4 | 43.918 | | | 1.00 39.94 | AAAA |
| MOTA | 22 N LYS A 5 | 44.332 | | | 1.00 40.39 | AAAA |
| ATOM | 23 CA LYS À 5 | 43.766 | | | 1.00 36.94 | AAAA |
| ATOM | 24 CB LYS A 5 | 44.142 45.179 | | | 1.00 34.10 | አጸጸጸ |
| ATOM | 25 CG LYS A 5 | | | | 1.00 35.02 | AAAA |
| ATOM | 26 CD LYS A 5 | 46.424 | | 65.698 | 1.00 34.07 | АААА |
| ATOM | 27 CE LYS A 5 | 47.233 | 40.452 | 65.652 | 1.00 33.44 | aaaa |
| ATOM | 28 NZ LYS A 5 | 48.565 49.372 | 40.239 | | 1.00 32.38 | AAAA |
| ATOM | 29 C LYS A 5 | 42.997 | 41.460 | 66.222 | 1.00 31.26 | aaaa |
| ATOM | 30 0 LYS A 5 | 42.053 | | 64.333 | 1.00 31.38 | AAAA |
| ATOM | 31 N LEUA 6 | 43.090 | 39.523 41.142 | 64.466 | 1.00 31.74 | AAAA |
| ATOM | 32 CA LEU A 6 | 42.075 | 41.142 | 63.326 | 1.00 28.60 | AAAA |
| ATOM | 33 CB LEU A 6 | 41.530 | | 62.289 | 1.00 26.90 | AAAA |
| ATOM | 34 CG LEU A 6 | 40.321 | 42.580 | 62.067 | 1.00 25.43 | AAAA |
| ATOM | 35 CD1 LEU A 6 | 40.108 | 42.748 44.224 | 61.129 | 1.00 25.89 | AAAA |
| ATOM | 36 CD2 LEU A 6 | 40.550 | 42.032 | 60.826 | 1.00 25.50 | AAAA |
| ATOM | 37 C LEU A 6 | 42.818 | 40.701 | 59.828 | 1.00 26.64 | AAAA |
| ATOM | 38 C LEU A 6 | 43.877 | 41.226 | 61.049 60.717 | 1.00 25.74 | AAAA |
| ATOM | 39 H ILE A 7 | 42.282 | 39.704 | 60.357 | 1.00 24.60 1.00 25.90 | AAAA |
| ATOM | 40 CA ILE A 7 | 42.939 | 39.212 | 59.173 | 1.00 26.75 | AAAA |
| ATOM | 41 CB ILE A 7 | 42.839 | 37.712 | 59.089 | 1.00 26.58 | λλλλ |
| ATOM | 42 CG2 ILE A 7 | 43.474 | 37.227 | 57.783 | 1.00 27.88 | AAAA |
| ATOM | 43 CG1 TLE A 7 | 43.528 | 37.116 | 60.310 | 1.00 27.02 | AAAA |
| ATOM | 44 CD1 TLE A 7 | 43.507 | 35.640 | 60.350 | 1.00 27.46 | AAAA |
| ATOM | 45 C ILE A 7 | 42.339 | 39.814 | 57.929 | 1.00 26.70 | AAAA |
| ATOM | 46 0 ILE A 7 | 41.162 | 39.655 | 57.681 | 1.00 27.68 | AAAA AAAA |
| ATOM | 47 N GLY A 8 | 43.144 | 40.509 | 57.142 | 1.00 27.94 | |
| ATCM | 48 CA GLY A 8 | 42.598 | 41.110 | 55.944 | 1.00 29.78 | AA A |
| ATOM | 49 C GLY A 8 | 43:.587 | 41.789 | 55.027 | 1.00 30.38 | AA. A |
| ATOM | 50 0 GLY A 8 | 44.785 | 41.765 | 55.264 | 1.00 29.39 | AAAA AAAA |
| ATOM | 51 N THR A 9 | 43.051 | 42.395 | 53.971 | 1.00 31.84 | AAAA |
| ATCM | 52 CA THR A 9 | 43.832 | 43.106 | 52.962 | 1.00 32.41 | |
| ATCM | 53 CB THR A 9 | 44.606 | 42.112 | 52.064 | 1.00 31.12 | AAAA AAAA |
| ATOM | 54 0G1 THR A 9 | 45.324 | 42.825 | 51.053 | 1.00 30.74 | AAAA |
| ATOM | 55 CG2 THR A 9 | 43.654 | 41.140 | 51.411 | 1.00 30.27 | AAAA |
| ATOM | 56 C THR A 9 | 42.886 | 43.939 | 52.091 | 1.00 32.94 | AAAA |
| ATOM | 57 3 THR A 9 | 41.705 | 43.625 | 51.993 | 1.00 33.62 | |
| ATOM | 58 N LEU A 10 | 43.396 | 45.009 | 51.485 | 1.00 33.02 | AAAA |
| ATOM | 59 CA LEU A 10 | 42.573 | 45.840 | 50.611 | 1.00 33.20 | AAAA |
| ATOM | 60 CB LEU A 10 | 43.117 | 47.275 | 50.484 | 1.00 33.29 | AAAA |
| ATCM | 51 CG LEU A 10 | 43.142 | 48.245 | 51.566 | 1.00 33.12 | AAAA |
| ATOM | 62 CD1 LEU A 10 | 41.743 | 48.386 | 52.288 | 1.00 31.99 | AAAA |
| ATOM | 63 CD2 LEU A 10 | 44.126 | 47.734 | 52.575 | 1.00 31.99 | AAAA |
| ATCM | 64 C LEU A 10 | 42.527 | 45.231 | 49.218 | 1.00 34.71 | AAAA |
| ATOM | 65 0 LEU A 10 | 41.876 | 45.768 | 48.328 | 1.00 33.18 | AAAA |
| ATCM | 66 N ASP A 11 | 43.230 | 44.121 | 49.022 | 1.00 32.52 | AAAA |
| | | | | | | AAAA, |

| MOTA | 67 | CA | ASP | A | 11 | 43.240 | 43.489 | 47.716 | 1.00 34.24 | AAAA |
|--------|-----|-----|-----|---|------|--------|--------|------------------|------------|---------------|
| MOTA | 68 | CB | ASP | Α | 11 | 44.393 | 42.499 | 47.607 | 1.00 35.81 | AAAA |
| MOTA | 69 | CG | ASP | A | 11 | 45.739 | 43.190 | 47.604 | 1.00 37.57 | AAAA |
| ATOM | 70 | | ASP | | 11 | 45.890 | 44.178 | 46.855 | 1.00 37.95 | AAAA |
| ATOM | 71 | | ASP | | 11 | 46.650 | 42.750 | 48.332 | 1.00 40.31 | AAAA |
| ATOM - | 72 | C | ASP | | 11 | 41.929 | 42.813 | 47.341 | 1.00 34.03 | AAAA |
| | 73 | ō | ASP | | 11 | 41.629 | 42.652 | 46.150 | 1.00 34.80 | AAAA |
| MOTA | | | TYR | | 12 | 41.142 | 42.417 | 48.335 | 1.00 32.34 | AAAA |
| ATOM | 74 | N | | | | | 41.803 | 48.017 | 1.00 32.53 | AAAA |
| MOTA | 75 | CA | TYR | | 12 | 39.871 | | | | |
| ATOM | 76 | СВ | TYR | | 12 | 39.043 | 41.569 | 49.290 | 1.00 31.32 | AAAA |
| MOTA | 77 | CG | TYR | | 12 | 39.551 | 40.438 | 50.162 | 1.00 29.95 | AAAA |
| MOTA | 78 | | TYR | | 12 | 39.983 | 40.669 | 51.469 | 1.00 28.52 | AAAA |
| MOTA | 79 | CE1 | TYR | A | 12 . | 40.413 | 39.614 | 52.279- | 1.00 28.03 | AAAA |
| MOTA | 80 | CD2 | TYR | A | 12 | 39.568 | 39.128 | 49.688 | 1.00 28.47 | AAAA |
| MOTA | 81 | CE2 | TYR | Α | 12 | 39.992 | 38.083 | 50.483 | 1.00 28.47 | AAAA |
| ATOM | 82 | CZ | TYR | Α | 12 | 40.408 | 38.330 | 51.775 | 1.00 28.43 | - AAAA |
| ATOM | 83 | OH | TYR | Α | 12 | 40.786 | 37.277 | 52.569 | 1.00 29.86 | AAAA |
| ATOM | 84 | С | TYR | Α | 12 | 39.146 | 42.749 | 47.066 | 1.00 33.16 | . AAAA |
| ATOM | 85 | ō | TYR | | 12 | 38.554 | 42.324 | 46.082 | 1.00 33.36 | AAAA |
| ATOM | 86 | N | GLY | | 13 | 39.237 | 44.041 | 47.356 | 1.00 34,76 | AAAA |
| ATOM | 87 | CA | GLY | | 13 | 38.594 | 45.065 | 46.546 | 1.00 36.60 | AAAA |
| ATOM | 88 | c | GLY | | 13 | 38.814 | 44.961 | 45.052 | 1.00 37.85 | AAAA |
| ATOM | 89 | ō | GLY | | 13 | 38.105 | 45.591 | 44.275 | 1.00 37.40 | AAAA |
| | 90 | N | LYS | | 14 | 39.799 | 44.171 | 44.647 | 1.00 39.55 | AAAA |
| MOTA | 91 | CA | LYS | | 14 | 40.091 | | 43.231 | 1.00 40.66 | AAAA |
| MOTA | | CB | LYS | | 14 | 41.605 | 43.977 | 42.995 | 1.00 42.26 | AAAA |
| MOTA | 92 | | LYS | | 14 | 42.300 | 45.309 | 43.239 | 1.00 44.54 | AAAA |
| MOTA | 93 | CG | LYS | | | 41.820 | 46.445 | 42.304 | 1.00 46.32 | AAAA |
| MOTA | 94 | CD | | | 14 | 42.033 | 46.158 | 40.810 | 1.00 46.64 | AAAA |
| MOTA | 95 | CE | LYS | | 14 | | | 40.256 | 1.00 47.23 | AAAA |
| MOTA | 96 | NZ | LYS | | 14 | 41.133 | 45.086 | | 1.00 40.35 | AAAA |
| ATOM | 97 | C | LYS | | 14 | 39.499 | 42.675 | 42.707 | | AAAA |
| ATOM | 98 | 0 | LYS | | 14 | 39.593 | 42.377 | 41.511 | 1.00 39.97 | |
| MOTA | 99 | N | TYR | | 15 | 38.897 | 41.901 | 43.605 | 1.00 39.95 | AAAA |
| MOTA | 100 | CA | TYR | | 15 . | 38.300 | 40.617 | 43.245 | 1.00 40.30 | AAAA |
| MOTA | 101 | CB | TYR | | 15 | 38.962 | 39.490 | 44.050 | 1.00 38.46 | AAAA |
| MOTA | 102 | CG | TYR | | 15 | 40.472 | 39.519 | 44.021 | 1.00 37.01 | AAAA |
| MOTA | 103 | | TYR | | 15 | 41.213 | 39.136 | 45.137 | 1.00 36.24 | AAAA |
| ATOM | 104 | CE1 | TYR | | 15 | 42.604 | 39.220 | 45.144 | 1.00 35.73 | AAAA |
| MOTA | 105 | CD2 | TYR | | 15 | 41.163 | 39.976 | 42.902 | 1.00 36.84 | AAAA |
| MOTA | 106 | CE2 | TYR | | 15 | 42.556 | 40.064 | 42.898 | 1.00 36.53 | AAAA |
| MOTA | 107 | CZ | TYR | A | 15 | 43.271 | 39.689 | 44.028 | 1.00 36.24 | AAAA |
| MOTA | 108 | OH | TYR | A | 15 | 44.648 | 39.816 | 44.042 | 1.00 36.49 | AAAA |
| ATOM | 109 | С | TYR | A | 15 | 36.802 | 40.647 | 43.556 | 1.00 41.98 | AAAA |
| ATOM | 110 | 0 | TYR | A | 15 | 36.288 | 39.786 | 44.280 | 1.00 42.59 | AAAA |
| ATOM | 111 | N | ARG | Α | 16 | 36.101 | 41.638 | 43.014 | 1.00 42.81 | · AAAA |
| ATOM | 112 | CA | ARG | Α | 16 | 34.670 | 41.753 | 43.257 | 1.00 43.47 | AAAA |
| ATOM | 113 | CB | ARG | Α | 16 | 34.205 | 43.197 | 43.111 | 1.00 45.27 | AAAA |
| ATOM | 114 | CG | ARG | A | 16 | 35.021 | 44.234 | 43.833 | 1.00 48.06 | AAAA |
| ATOM | 115 | CD | ARG | Α | 16 | 34.891 | 44.196 | 45.339 | 1.00 49.63 | AAAA |
| ATOM | 116 | NE | ARG | Α | 16 | 35.632 | 45.322 | 45.905 | 1.00 51.65 | AAAA |
| ATOM | 117 | CZ | ARG | | 16 | 35.382 | 46.602 | 45.622 | 1.00 52.71 | AAAA |
| ATOM | 118 | | ARG | | 16 | 34.406 | 46.931 | 44.781 | 1.00 53.28 | AAAA |
| ATOM | 119 | | ARG | | 16 | 36.124 | 47.560 | 46.162 | 1.00 53.43 | AAAA |
| | 120 | C | ARG | | 16 | 33.913 | 40.929 | 42.230 | 1.00 42.86 | AAAA |
| ATOM | 121 | ō | ARG | | 16 | 34.455 | 40.541 | 41.193 | 1.00 41.83 | AAAA |
| ATOM | | N | TYR | | 17 | 32.651 | 40.668 | 42.523 | 1.00 42.42 | · AAAA |
| ATOM | 122 | | TYR | | 17 | 31.818 | 39.942 | 41.590 | 1.00 42.76 | AAAA |
| ATOM | 123 | CA | | | 17 | 30.675 | 39.254 | 42.333 | 1.00 40.11 | AAAA |
| ATOM | 124 | CB | TYR | | | 31.097 | 38.061 | 43.180 | 1.00 38.35 | AAAA |
| MOTA | 125 | CG | TYR | | 17 | | 38.148 | 44.071 | 1.00 36.15 | AAAA |
| ATOM | 126 | CD1 | | | 17 | 32.169 | | | 1.00 34.76 | AAAA |
| ATOM | 127 | CE1 | TYR | | 17 | 32.519 | 37.069 | 44.874 43.116 | 1.00 36.40 | AAAA |
| MOTA | 128 | CD2 | TYR | | 17 | 30.386 | 36.855 | | 1.00 35.31 | AAAA |
| MOTA | 129 | CE2 | TYR | | 17 | 30.726 | 35.776 | 43.912 | 1.00 35.31 | AAAA |
| MOTA | 130 | CZ | TYR | | 17 | 31.792 | 35.887 | 44.790 | T.00 33.00 | AAAA |
| ATOM | 131 | OH | TYR | | 17 | 32.115 | 34.814 | 45.584 | 1.00 33.29 | |
| MOTA | 132 | С | TYR | Α | 17 | 31.296 | 41.000 | 40.613 | 1.00 44.43 | AAAA |

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| MOTA | 133 | 0 | TYR | A 17 | 31.346 | 42.194 | 40.905 | 1.00 44.68 | AAAA |
|------|-----|------|---------|------|-----------|------------------|------------------|--------------------------|--------------|
| MOTA | 134 | N | PRO | A 18 | 30.799 | | | | AAAA |
| MOTA | 135 | CI | PRO | A 18 | 30.707 | | | | AAAA |
| MOTA | 136 | C.P. | PRO | | 30.268 | | | | AAAA |
| ATOM | 137 | CE | PRO | | 29.854 | | | | AAAA |
| ATOM | 138 | CG | PRO | A 18 | 30.876 | | | | AAAA |
| ATOM | 139 | С | PRO | | 29.129 | | | | AAAA |
| ATOM | 140 | | PRO | | 28.298 | | | | . AAAA |
| ATOM | 141 | | LYS | | 29.114 | | | | |
| ATOM | 142 | | | | 28.125 | | | | AAAA |
| ATOM | 143 | CB | | | 27.876 | | | | AAAA |
| ATOM | 144 | CG | | | 29.120 | | | | AAAA |
| ATOM | 145 | | | | 28.747 | | | | AAAA |
| ATOM | 146 | CE | | | 29.978 | | | | AAAA |
| ATOM | 147 | NZ | | | 29.616 | | | 1.00 61.03 | AAAA |
| ATOM | 148 | c | LYS | | 26.764 | | | 1.00 51.53 | AAAA |
| ATOM | 149 | ō | LYS | | 26.281 | | | 1.00 51.53 | AAAA |
| ATOM | 150 | N | ASN . | | 26.146 | | | | AAAA |
| ATOM | 151 | CA | | | 24.831 | 42.750 | | 1.00 50.13 | AAAA |
| ATOM | 152 | CB | ASN | | 24.336 | | | 1.00 48.44 | AAAA |
| ATOM | 153 | CG. | | | 25.389 | 41.132 | 36.613 | 1.00 49.67 | AAAA |
| MOTA | 154 | | l ASN | | 25.677 | | | 1.00 51.61 | AAAA |
| ATOM | 155 | | 2 ASN A | | 25.998 | 41.562 | 35.509 | 1.00 51.70 | AAAA |
| ATOM | 156 | C | ASN A | | 24.789 | | | 1.00 53.00 | AAAA |
| ATOM | 157 | õ | ASN A | | 23.764 | 41.765 41.127 | 39.649 | 1.00 45.57 | AAAA |
| ATOM | 158 | N | HIS A | | 25.883 | 41.127 | 39.877 40.398 | 1.00 44.67 | AAAA |
| ATOM | 159 | CA | HIS A | | 25.958 | 40.709 | 41.506 | 1.00 42.71 | AAAA |
| ATOM | 160 | CB | HIS A | | 27.216 | 39.857 | 41.353 | 1.00 40.69 1.00 40.16 | AAAA |
| ATOM | 161 | CG | HIS A | | 27.210 | 38.587 | 42.140 | 1.00 40.16 | AAAA |
| ATOM | 162 | | HIS A | | 27.329 | 38.353 | 43.467 | 1.00 39.33 | AAAA |
| ATOM | 163 | | HIS A | | 26.951 | 37.359 | 41.557 | 1.00 39.27 | AAAA |
| ATOM | 164 | | HIS A | | 26.948 | 36.425 | 42.493 | 1.00 39.36 | AAAA |
| ATOM | 165 | | HIS A | | 27.174 | 37.003 | | 1.00 39.44 | AAAA |
| MOTA | 166 | C | HIS A | | 25.974 | 41.349 | 42.892 | 1.00 38.93 | AAAA AAAA |
| ATOM | 167 | ō | HIS A | | 26.660 | 42.338 | 43.116 | 1.00 38.78 | AAAA |
| ATOM | 168 | N | PRO A | | 25.229 | 40.778 | 43.853 | 1.00 37.11 | AAAA |
| ATOM | 169 | CD | PRO A | - | 24.371 | 39.579 | 43.814 | 1.00 36.09 | AAAA |
| ATOM | 170 | CA | PRO A | | 25.224 | 41.361 | 45.199 | 1.00 35.81 | AAAA |
| ATOM | 171 | CB | PRO A | | 24.473 | 40.306 | 46.012 | 1.00 36.04 | AAAA |
| ATOM | 172 | CG | PRO A | | 23.464 | 39.810 | 45.003 | 1.00 36.19 | AAAA |
| ATOM | 173 | C | PRO A | | 26.638 | 41.637 | 45.751 | 1.00 34.39 | AAAA |
| ATOM | 174 | O | PRO A | | 26.867 | 42.653 | 46.417 | 1.00 34.09 | AAAA |
| ATOM | 175 | N | LEU A | | 27.572 | 40.731 | 45.451 | 1.00 31.98 | AAAA |
| ATOM | 176 | CA | LEU A | | 28.954 | 40.827 | 45.900 | 1.00 29.65 | AAAA |
| ATOM | 177 | CB | LEU A | | 29.564 | 39.432 | 46.014 | 1.00 27.88 | AAAA |
| ATOM | 178 | CG | LEU A | | 28.896 | 38.528 | 47.048 | 1.00 27.31 | AAAA |
| ATOM | 179 | CD1 | LEU A | 23 | 29.656 | 37.217 | 47.149 | 1.00 26.64 | AAA |
| ATOM | 180 | CD2 | LEU A | 23 | 28.879 | 39.212 | 48.399 | 1.00 26.75 | AAAA |
| ATOM | 181 | С | LEU A | 23 | 29.838 | | 45.018 | 1.00 29.20 | AAAA |
| ATOM | 182 | 0 | LEU A | 23 | 31.057 | 41.606 | 45.028 | 1.00 28.38 | AAAA |
| MOTA | 183 | N | LYS A | 24 | 29.204 | 42.582 | 44.259 | 1.00 29.27 | AAAA |
| ATOM | 184 | CA | LYS A | 24 | 29.903 | 43.512 | | . 1.00 29.30 | AAAA |
| MOTA | 185 | CB | LYS A | 24 | 28.881 | 44.091 | 42.405 | 1.00 29.75 | AAAA |
| ATOM | 186 | CG | LYS A | 24 | 29.328 | 45.265 | 41.601 | 1.00 32.55 | AAAA |
| ATOM | 187 | CD | LYS A | 24 | 28.537 | 46.526 | 41.994 | 1.00 34.37 | AAAA |
| MOTA | 188 | CE | LYS A | 24 | 27.025 | 46.337 | 41.835 | 1.00 34.32 | AAAA |
| ATOM | 189 | NZ | LYS A | 24 | 26.221 | 47.542 | 42.208 | 1.00 34:37 | AAAA |
| ATOM | 190 | С | LYS A | 24 | 30.580 | 44.620 | 44.224 | 1.00 28.14 | AAAA |
| ATOM | 191 | 0 | LYS A | 24 | 31.617 | 45.162 | 43.840 | 1.00 27.93 | AAAA |
| ATOM | 192 | N | ILE A | 25 | 29.990 | 44.919 | 45.377 | 1.06 27.07 | AAAA |
| ATOM | 193 | CA | ILE A | 25 | 30.468 | 45.945 | 46.296 | 1.00 25.82 | AAAA |
| ATOM | 194 | СВ | ILE A | 25 | 29.425 | 46.262 | 47.364 | 1.00 25.37 | AAAA |
| ATOM | 195 | | ILE A | 25 | 28.190 | 46.846 | 46.737 | 1.00 25.71 | AAAA |
| ATOM | 196 | | ILE A | 25 | 29.142 | 44.979 | 48.157 | 1.00 25.26 | AAAA |
| ATOM | | | ILE A | 25 | 28.318 | 45.163 | 49.413 | 1.00 25.17 | AAAA |
| ATOM | | C | ILE A | 25 | 31.700 | 45.550 | 47.095 | 1.00 25.28 | , AAAA |
| | | - | | | + · · · · | | | _,_, | |



| - 51016 | 100 | ^ | ILE A | 25 | 32.037 | 44.379 | 47.183 | 1.00 24.48 | AAAA · |
|---------|-------|-----|-------|-----|--------|--------|--------|------------|--------|
| MOTA | 199 | 0 | | | | | | | |
| ATOM | 200 | Я | PRO A | 26 | 32.375 | 46.547 | 47.714 | 1.00 24.98 | AAAA |
| ATOM | 201 | CD | PRO A | 26 | 32.062 | 47.980 | 47.638 | 1.00 24.98 | AAAA |
| ATOM | 202 | CA | PRO A | 26 | 33.570 | 46.367 | 48.543 | 1.00 24.44 | AAAA |
| | | CB | PRO A | 26 | 34.094 | 47.792 | 48.701 | 1.00 24.75 | AAAA |
| MOTA | 203 | | | | | | | 1.00 25.51 | |
| MOTA | 204 | CG | PRO A | 26 | 33.435 | 48.546 | 47.538 | | AAAA |
| MOTA | 205 | С | PRO A | 26 | 33.021 | 45.838 | 49.862 | 1.00 23.42 | AAAA |
| | 206 | 0 | PRO A | 26 | 31.930 | 46.233 | 50.272 | 1.00 22.12 | AAAA |
| ATOM | | | | | 33.754 | 44.960 | 50.532 | 1.00 23.06 | AAAA |
| MOTA | 207 | N | ARG A | 27 | | | | | |
| ATOM | 208 | CA | ARG A | 27 | 33.244 | 44.421 | 51.776 | 1.00 23.04 | AAAA |
| MOTA | 209 | CB | ARG A | 27 | 32.633 | 43.043 | 51.492 | 1.00 22.20 | AAAA |
| | 210 | CG | ARG A | 27 | 31.463 | 43.152 | 50.503 | 1.00 19.84 | AAAA |
| MOTA | | | | | 30.762 | 41.844 | 50.160 | 1.00 18.64 | AAAA |
| MOTA | 211 | CD | ARG A | 27 | | | | | |
| ATOM | 212 | NE | ARG A | 27 | 30.181 | 41.168 | 51.315 | 1.00 16.51 | AAAA |
| ATOM | 213 | CZ | ARG A | 27 | 30.774 | 40.188 | 51.982 | 1.00 16.57 | AAAA |
| | 214 | | ARG A | 27 | 31.969 | 39.763 | 51.605 | 1.00 17.50 | AAAA ' |
| MOTA | | | | 27 | 30.185 | 39.643 | 53.038 | 1.00 16.45 | AAAA |
| MOTA | 215 | NHZ | ARG A | | | | | | |
| MOTA | 216 | C | ARG A | 27 | 34.265 | 44.381 | 52.905 | 1.00 23.62 | AAAA |
| MOTA | 217 | 0 | ARG A | 27 | 34.107 | 45.077 | 53.919 | 1.00 23.69 | AAAA |
| | 218 | N | VAL A | 28 | 35.305 | 43.570 | 52.736 | 1.00 24.25 | AAAA |
| MOTA | | | | | | 43.466 | 53.737 | 1.00 23.36 | AAAA |
| MOTA | 219 | CA | VAL A | 28 | 36.355 | | | | |
| ATOM | 220 | CB | VAL A | 28 | 37.022 | 42.062 | 53.671 | 1.00 22.75 | AAAA |
| ATOM | 221 | CG1 | VAL A | 28 | 38.292 | 42.031 | 54.475 | 1.00 22.95 | AAAA |
| | 222 | | VAL A | 28 | 36.061 | 41.011 | 54.249 | 1.00 22.20 | AAAA |
| MOTA | | | | | 37.363 | 44.609 | 53.511 | 1.00 23.70 | AAAA |
| ATOM | . 223 | С | VAL A | 28 | | | | | |
| MOTA | 224 | 0 | VAL A | 28 | 37.943 | 45.156 | 54.455 | 1.00 22.62 | AAAA |
| ATOM | 225 | N | SER A | 29 | 37.538 | 44.989 | 52.253 | 1.00 24.27 | AAAA |
| | 226 | CA | SER A | 29 | 38.444 | 46.082 | 51.910 | 1.00 26.03 | AAAA |
| ATOM | | | | 29 | 38.632 | 46.178 | 50.381 | 1.00 25.95 | AAAA |
| MOTA | 227 | CB | SER A | | | | | | |
| ATOM | 228 | 0G | SER A | 29 | 37.395 | 46.417 | 49.716 | 1.00 27.57 | AAAA |
| MOTA | 229 | C | SER A | 29 | 37.793 | 47.354 | 52.440 | 1.00 25.52 | aaaa |
| | 230 | ō | SER A | 29 | 38.463 | 48.311 | 52.828 | 1.00 25.49 | AAAA |
| MOTA | | | | 30 | 36.468 | 47.342 | 52.448 | 1.00 26.09 | AAAA |
| ATOM | 231 | N | LEU A | | | | | 1.00 26.39 | AAAA |
| MOTA | 232 | CA | LEU A | 30 | 35.692 | 48.471 | 52.926 | | |
| ATOM | 233 | CB | LEU A | 30 | 34.262 | 48.365 | 52.393 | 1.00 25.89 | AAAA |
| ATOM | 234 | CG | LEU A | 30 | 33.265 | 49.470 | 52.755 | 1.00 27.15 | AAAA |
| | | | LEU A | 30 | 32.486 | 49.101 | 53.999 | 1.00 26.34 | AAAA |
| MOTA | 235 | | | | _ | 50.813 | 52.897 | 1.00 25.81 | AAAA |
| MOTA | 236 | CD2 | LEU A | 30 | 34.015 | | | | |
| MOTA | 237 | С | LEU A | 30 | 35.713 | 48.534 | 54.453 | 1.00 26.26 | AAAA |
| ATOM | 238 | 0 | LEU A | 30 | 35.731 | 49.612 | 55.037 | 1.00 27.50 | AAAA |
| | 239 | N | LEU A | 31 | 35.730 | 47.379 | 55.097 | 1.00 25.57 | AAAA |
| ATOM | | | | 31 | 35.776 | 47.343 | 56.545 | 1.00 26.87 | AAAA |
| MOTA | 240 | CA | LEU A | | | | 57.029 | 1.00 27.28 | AAAA |
| ATOM | 241 | CB | LEU A | 31 | 35.752 | 45.900 | | | |
| MOTA | 242 | CG | LEU A | 31 | 35.135 | 45.563 | 58.383 | 1.00 27.87 | AAAA |
| ATOM | 243 | CD1 | LEU A | 31 | 35.855 | 44.313 | 58.906 | 1.00 27.01 | AAAA |
| - | | | LEU A | 31 | 35 261 | 46.706 | 59.372 | 1.00 26.32 | AAAA |
| ATOM | 244 | | | | 37.087 | 48.003 | 57.012 | 1.00 28.08 | AAAA |
| MOTA | 245 | С | LEU A | 31 | | | | | |
| MOTA | 246 | 0 | LEU A | 31 | 37 094 | 48.854 | 57.901 | 1.00 27.42 | AAAA |
| ATOM | 247 | N | LEU A | 32 | 38.197 | 47.584 | 56.409 | 1.00 29.52 | AAAA |
| | 248 | CA | LEU A | 32 | 39.508 | 48.121 | 56.750 | 1.00 30.96 | AAAA |
| MOTA | | | | | 40.607 | 47.394 | 55.950 | 1.00 31.58 | AAAA |
| ATOM | 249 | CB | LEU A | | | | | | AAAA |
| ATOM | 250 | CG | LEU A | 32 | 40.792 | 45.904 | 56.293 | 1.00 31.63 | |
| ATOM | 251 | CDI | LEU A | 32 | 41.810 | 45.246 | 55.380 | 1.00 31.31 | AAAA |
| | | CD2 | LEU A | 32 | 41.232 | 45.780 | 57.743 | 1.00 32.23 | AAAA |
| MOTA | 252 | | | | | | 56.543 | 1.00 31.59 | AAAA |
| ATOM | 253 | C | LEU A | 32 | 39.599 | 49.635 | | | |
| ATOM | 254 | 0 | LEU A | 32 | 40.081 | 50.345 | 57.416 | 1.00 31.70 | AAAA |
| ATOM | 255 | N | ARG A | 33 | 39.140 | 50.129 | 55.398 | 1.00 32.72 | AAAA |
| | • | | ARG A | 33 | 39.178 | 51.564 | 55.141 | 1.00 33.91 | AAAA |
| ATOM | 256 | CA | | | | | 53.743 | 1.00 35.10 | AAAA |
| ATOM | 257 | CB | ARG A | | 38.643 | 51.903 | | | |
| ATOM | 258 | CG | ARG A | 33 | 39.627 | 51.609 | 52.621 | 1.00 37.84 | AAAA |
| | 259 | CD | ARG A | 33 | 39.310 | 52.412 | 51.374 | 1.00 39.33 | aaaa |
| ATOM | | | ARG A | 33 | 38.255 | 51.806 | 50.580 | 1.00 42.51 | AAAA |
| ATOM | 260 | NE | | | | | 49.541 | 1.00 44.22 | AAAA |
| ATOM | 261 | CZ | ARG A | | 37.662 | 52.395 | | | |
| ATOM | 262 | NHl | ARG A | 33 | 38.016 | | 49.163 | 1.00 44.61 | AAAA |
| | 263 | NH2 | ARG A | 33 | 36.723 | 51.752 | 48.861 | 1.00 45.23 | AAAA |
| ATOM | | | ARG A | 33 | 38.352 | 52.305 | 56.168 | 1.00 33.48 | AAAA |
| atcm | 264 | С | ANG N | 7.3 | 242 | 22.303 | - | | |
| • | | | | | | | | | • |

| ATOM | 265 | 0 | ARG A | 33 | | 38.713 | 53.390 | 56.592 | 1.00 33.61 | AAAA |
|--------|-------|-----|-------|----|---|--------|-----------------|--------|------------|-------------|
| MOTA | 266 | · N | PHE A | 34 | | 37.247 | 51.682 | 56.562 | 1.00 33.78 | AAAA |
| | | | | 34 | | | | | | |
| MOTA | 267 | CA | PHE A | | | 36.292 | 52.233 | 57.517 | 1.00 33.79 | AAAA |
| MOTA | 268 | CB | PHE A | 34 | | 35.065 | 51.310 | 57.573 | 1.00 33.88 | AAAA |
| ATOM | 269 | CG | PHE A | 34 | | 33.925 | 51.840 | 58.405 | 1.00 33.16 | AAAA |
| ATOM | 270 | | PHE A | 34 | | 33.108 | 52.856 | 57.925 | 1.00 32.77 | AAAA |
| | | | | | | | | | | |
| atom | 271 | | PHE A | 34 | | 33.668 | 51.315 | 59.672 | 1.00 33.05 | AAAA |
| MOTA | 272 | CE1 | PHE A | 34 | • | 32.044 | 53.343 | 58.695 | 1.00 32.86 | AAAA |
| ATOM | 273 | CE2 | PHE A | 34 | | 32.607 | 51.797 | 60.454 | 1.00 33.07 | AAAA |
| | | | | | | | | | | |
| MOTA | 274 | CZ | PHE A | 34 | | 31.794 | 52.809 | 59.966 | 1.00 32.58 | AAAA |
| MOTA | 275 | С | PHE A | 34 | - | 36.881 | 52.414 | 58.918 | 1.00 34.01 | . AAAA |
| MOTA | 276 | 0 | PHE A | 34 | | 36.903 | 53.524 | 59.455 | 1.00 33.49 | AAAA |
| | 277 | N | LYS A | 35 | | 37.350 | 51.324 | 59.516 | 1.00 34.00 | AAAA |
| ATOM | | | | | | | | | | |
| MOTA | 278 | CA | LYS A | 35 | | 37.928 | 51.401 | 60.843 | 1.00 33.90 | AAAA |
| ATOM | 279 | CB | LYS A | 35 | | 38.230 | 50.010 | 61.362 | 1.00 34.07 | AAAA |
| ATOM | 280 | CG | LYS A | 35 | | 37.000 | 49.190 | 61.662 | 1.00 33.94 | AAAA |
| | | | | | | | | | | |
| MOTA | 281 | CD | LYS A | 35 | | 37.414 | 47.810 | 62.106 | 1.00 35.31 | AAAA |
| ATOM | 282 | CE | LYS A | 35 | | 38.062 | 47.072 | 60.948 | 1.00 35.91 | AAAA |
| ATOM | 283 | NZ | LYS A | 35 | | 39.058 | 47.928 | 60.236 | 1.00 36.19 | AAAA |
| | 284 | C | LYS A | 35 | | 39.185 | 52.255 | 60.881 | 1.00 34.19 | AAAA |
| ATOM | | | | | | | | | | |
| MOTA | 285 | 0 | LYS A | 35 | | 39.554 | 52.775 | 61.929 | 1.00 34.32 | AAAA |
| ATOM | 286 | N | ASP A | 36 | | 39.853 | 52.384 | 59.745 | 1.00 33.99 | AAAA |
| ATOM | 287 | CA | ASP A | 36 | | 41.034 | 53.216 | 59.680 | 1.00 35.17 | AAAA |
| MOTA | | | ASP A | 36 | | 41.812 | 52.943 | 58.388 | 1.00.37.40 | AAAA |
| | 288 | CB | | | | | | | | |
| MOŢA | 289 | CG | ASP A | 36 | | 42.964 | 53.908 | 58.186 | 1.00 38.64 | AAAA |
| ATOM | 290 | OD1 | ASP A | 36 | | 43.648 | 54.218 | 59.184 | 1.00 40.02 | AAAA |
| ATOM | 291 | 002 | ASP A | 36 | | 43.201 | 54.341 | 57.035 | 1.00 38.74 | AAAA |
| | | | ASP A | 36 | | 40.568 | 54.670 | 59.724 | 1.00 35.85 | AAAA |
| MOTA | 292 | C | | | • | | | | | |
| ATOM | 293 | 0 | ASP A | 36 | | 41.231 | 55.527 | 60.306 | 1.00 36.88 | AAAA |
| -MOTA | 294 | N | ALA A | 37 | | 39.420 | 54.940 | 59.111 | 1.00 34.96 | AAAA |
| ATOM | 295 | CA | ALA A | 37 | | 38.851 | 56.280 | 59.108 | 1.00 34.47 | AAAA |
| | | | | | | | 56.373 | | | |
| ATOM | 296 | CB | ALA A | 37 | | 37.751 | | 58.067 | 1.00 33.80 | AAAA |
| ATOM | 297 | С | ALA A | 37 | | 38.291 | 56.617 | 60.499 | 1.00 34.66 | AAAA |
| ATOM | 298 | 0 | ALA A | 37 | | 38.268 | 57. 77 9 | 60.899 | 1.00 34.55 | AAAA |
| ATOM | 299 | N | MET A | 38 | | 37.830 | 55.600 | 61.226 | 1.00 34.24 | AAAA |
| | | | | | | | 55.794 | 62.572 | 1.00 33.07 | AAAA |
| MOTA | 300 | CA | MET A | 38 | | 37.287 | | | | |
| MOTA | 301 | CB | MET A | 38 | | 36.289 | 54.687 | 62.917 | 1.00 32.82 | AAAA |
| ATOM | 302 | CG | MET A | 38 | | 35.084 | 54.559 | 61.996 | 1.00 32.72 | AAAA |
| ATOM | 303 | SD | MET A | 38 | | 33.980 | 55.948 | 62.101 | 1.00 33.65 | AAAA |
| | | | | 38 | | | 55.878 | | 1.00 33.77 | AAAA |
| ATOM | . 304 | CE | MET A | | | 33.550 | | 63.849 | | |
| ATOM . | 305 | С | MET A | 38 | | 38.430 | 55.724 | 63.583 | 1.00 33.12 | AAAA |
| MOTA | 306 | 0 | MET A | 38 | | 38.226 | 55.930 | 64.777 | 1.00 32.82 | AAAA |
| ATOM | 307 | N | ASN A | 39 | | 39.628 | 55.428 | 63.090 | 1.00 32.64 | AAAA |
| | | | | | | | | | 1.00 32.38 | AAAA |
| ATOM | 308 | CA | ASN A | 39 | | 40.805 | 55.266 | 63.935 | | |
| ATOM | 309 | CB | ASN A | 39 | | 41.200 | 56.600 | 64.589 | 1.00 32.93 | AAAA |
| MOTA | 310 | CG | ASN A | 39 | | 41.393 | 57.736 | 63.571 | 1.00 34.40 | AAAA |
| ATOM | 311 | | ASN A | 39 | • | 42.180 | 57.624 | 62.630 | 1.00 34.98 | AAAA |
| | | | | | | | _ | | 1.00 33.52 | |
| ATOM | 312 | | ASN A | 39 | | 40.677 | 58.838 | 63.772 | | AAAA |
| MOTA | 313 | С | asn a | 39 | • | 40.483 | 54.212 | 65.009 | 1.00 31.69 | AAAA |
| ATOM | 314 | 0 | ASN A | 39 | | 40.565 | 54.490 | 66.205 | 1.00 31.12 | AAAA |
| | | | | 40 | | 40.095 | 53.010 | 64.570 | 1.00 31.76 | AAAA |
| ATOM | 315 | N | LEU A | | | | | | | |
| MOTA | 316 | CA | LEU A | 40 | | 39.750 | 51.898 | 65.474 | 1.00 32.48 | AAAA |
| ATOM | 317 | CB | LEU A | 40 | | 38.259 | 51.559 | 65.386 | 1.00 32.55 | AAAA |
| ATOM | .318 | CG | LEU A | 40 | | 37.231 | 52.581 | 65.879 | 1.00 32.84 | AAAA |
| | | | | | | 35.837 | 52.089 | 65.554 | 1.00 33.79 | AAAA |
| ATOM | 319 | | LEU A | 40 | | | | | | |
| MOTA | 320 | CD2 | LEU A | 40 | | 37.372 | 52.798 | 67.376 | 1.00 32.45 | AAAA |
| MOTA | 321 | С | LEU A | 40 | | 40.555 | 50.628 | 65.187 | 1.00 32.92 | AAAA |
| | | | | 40 | | 40.196 | 49.530 | 65.618 | 1.00 31.64 | AAAA |
| ATOM | 322 | 0 | LEU A | | | | | | 1.00 34.12 | |
| MOTA | 323 | N | ILE A | 41 | | 41.652 | 50.794 | 64.464 | | AAAA |
| MOTA | 324 | CA | ILE A | 41 | | 42.508 | 49.680 | 64.116 | 1.00 36.07 | AAAA |
| ATOM | 325 | CB | ILE A | 41 | | 42.017 | 48.991 | 62.811 | 1.00 35.51 | AAAA |
| | | | | | | 42.070 | 49.952 | 61.636 | 1.00 33.37 | AAAA |
| ATOM | 326 | | ILE A | 41 | | | | | 1.00 35.97 | |
| ATOM | 327 | | ILE A | 41 | | 42.898 | 47.790 | 62.480 | 1.00 33.37 | AAAA |
| MOTA | 328 | CD1 | ILE A | 41 | • | 42.854 | 46.701 | 63.500 | 1.00 37.19 | AAAA |
| | 329 | c | ILE A | 41 | | 43.921 | 50.226 | 63.916 | 1.00 38.85 | AAAA |
| ATOM | | | | | | | | | 1.00 38.98 | AAAA |
| MOTA | 330 | 0 | ILE A | 41 | | 44.106 | 51.346 | 63.413 | 1.00 50.50 | · remain |

| ATOM | 331 | N | ASP | Α | 42 | 4 | 14.914 | 49.446 | 64.329 | 1.00 | 40.61 | AAAA |
|-------|-----|-----|------------|----|----|------|--------|--------|--------|------|-------|--------|
| ATOM | 332 | CA | AŞP | 2 | 42 | | 16.309 | 49.843 | 64.181 | | 42.57 | |
| | | | | | | | | | | | | AAAA |
| ATOM | 333 | | ASP | | 42 | | 16.973 | 50.021 | 65.553 | 1.00 | 42.42 | AAAA |
| ATOM | 334 | CG | ASP | Α | 42 | 4 | 16.316 | 51.110 | 66.381 | 1.00 | 42.27 | AAAA |
| ATOM | 335 | OD: | l ASP | Α | 42 | 4 | 16.227 | 52.250 | 65.883 | | 41.20 | AAAA |
| ATOM. | 336 | | 2 ASP | | 42 | | 5.891 | 50.833 | 67.526 | | | |
| | | | | | | | | | | | 43.36 | AAAA |
| ATOM | 337 | C | ASP | | 42 | | 17.011 | 48.752 | 63.392 | | 44.05 | AAAA |
| ATOM | 338 | 0 | ASP | Α | 42 | 4 | 6.525 | 47.620 | 63.333 | 1.00 | 44.88 | `AAAA |
| ATOM | 339 | N | GLU | Α | 43 | 4 | 8.147 | 49.090 | 62.789 | | 45.10 | AAAA |
| ATOM | 340 | CA | _GLU | | 43 | | | | | | | |
| | | | | | | | 8.905 | 48.141 | 61.980 | | 46.11 | AAAA |
| ATOM | 341 | CB | GLU | | 43 | 5 | 0.172 | 48.796 | 61.454 | 1.00 | 46.89 | AAAA |
| MOTA | 342 | CG | GLU | A. | 43 | 4 | 9.924 | 50.057 | 60.668 | 1.00 | 49.30 | AAAA |
| ATOM | 343 | CD | GLU | A | 43 | - 5 | 1.187 | 50.580 | 60.028 | | 49.67 | |
| ATOM | 344 | | GLU | | | | | | | | | AAAA |
| | | | | | 43 | | 1.760 | 49.839 | 59.201 | | 50.60 | AAAA |
| MOTA | 345 | | : GLU | | 43 | 5 | 1.601 | 51.714 | 60.349 | | 49.60 | AAAA |
| ATOM | 346 | С | GLU | A | 43 | 4 | 9.290 | 46.859 | 62.701 | 1.00 | 46.27 | - AAAA |
| MOTA | 347 | 0 | GLU | Α | 43 | 4 | 9.214 | 45.773 | 62.131 | | 46.00 | AAAA |
| ATOM | 348 | N | LYS | | 44 | | 9.708 | 46.986 | 63.954 | | | |
| | | | | | | | | | | | 46.52 | AAAA |
| MOTA | 349 | CA | LYS | | 44 | | 0.135 | 45.832 | 64.730 | | 46.31 | AAAA |
| ATOM | 350 | CB | LYS | Α | 44 | 5 | 0.762 | 46.306 | 66.048 | 1.00 | 48.16 | AAAA |
| MOTA | 351 | CG | LYS | Α | 44 | 5 | 1.977 | 47.215 | 65.799 | | 51.59 | AAAA |
| ATOM | 352 | CD | LYS | | 44 | | 2.641 | 47.734 | 67.071 | | | |
| | | • | | | | | | | | | 52.87 | AAAA |
| ATOM | 353 | CE | LYS | | 44 | | 3.851 | 48.601 | 66.727 | 1.00 | 53.34 | AAAA |
| ATOM | 354 | NZ | LYS | Α | 44 | 5 | 4.615 | 49.033 | 67.936 | 1.00 | 53.45 | AAAA |
| ATOM | 355 | С | LYS | Α | 44 | 4 | 9.029 | 44.828 | 64.996 | 1.00 | 44.74 | AAAA |
| ATOM | 356 | 0 | LYS | | 44 | | 9.296 | 43.735 | 65.480 | | 45.35 | |
| ATOM | 357 | N | GLU | | | | | | | | | AAAA |
| | | | | | 45 | | 7.793 | 45.190 | 64.659 | | 42.49 | AAAA |
| MOTA | 358 | CA | GLU | | 45 | 4 | 6.638 | 44.320 | 64.894 | 1.00 | 40.54 | AAAA |
| MOTA | 359 | CB | GLU | A. | 45 | 4. | 5.493 | 45.125 | 65.517 | 1.00 | 40.55 | AAAA |
| ATOM | 360 | CG | GLU | Α | 45 | 4 | 5.788 | 45.731 | 66.882 | | 38.87 | AAAA |
| ATOM | 361 | CD | GLU | | 45 | | 4.663 | 46.618 | 67.360 | | | |
| | | | | | | | | | | | 37.57 | AAAA |
| MOTA | 362 | | GLU | | 45 | | 4.383 | 47.631 | 66.693 | | 36.29 | AAAA |
| ATOM | 363 | OE2 | ${	t GLU}$ | A | 45 | 4. | 4.056 | 46.300 | 68.399 | 1.00 | 38.44 | AAAA |
| ATOM | 364 | С | GLU | Α | 45 | 4 | 6.126 | 43.648 | 63.630 | 1.00 | 39.15 | AAAA |
| ATOM | 365 | 0 | GLU | | 45 | | 5.301 | 42.737 | 63.681 | | 39.29 | AAAA |
| ATOM | 366 | N | LEU | | 46 | | 6.619 | 44.115 | 62.497 | | | |
| | | | | | | | | | | | 37.62 | AAAA |
| ATOM | 367 | CA | LEU | | 46 | | 6.219 | 43.589 | 61.211 | 1.00 | 35.88 | AAAA |
| MOTA | 368 | CB | LEU | A | 46 | 4 | 6.125 | 44.750 | 60.229 | 1.00 | 36.09 | AAAA |
| MOTA | 369 | CG | LEU | Α | 46 | 4. | 5.608 | 44.550 | 58.817 | 1.00 | 36.50 | AAAA |
| ATOM | 370 | CD1 | LEU | | 46 | | 4.182 | 44.021 | 58.843 | | 36.66 | |
| MOTA | 371 | | LEU | | | | | | | | | AAAA |
| | | | | | 46 | | 5.646 | 45.893 | 58.113 | | 35.85 | AAAA |
| ATOM | 372 | С | LEU . | | 46 | | 7.211 | 42.542 | 60.714 | 1.00 | 34.97 | AAAA |
| MOTA | 373 | 0 | LEU | A | 46 | 48 | 3.424 | 42.670 | 60.900 | 1.00 | 35.72 | AAAA |
| ATOM | 374 | N | ILE . | A | 47 | 46 | 5.680 | 41.484 | 60.118 | 1.00 | 33.25 | AAAA |
| ATOM | 375 | CA | ILE | | 47 | | 7.497 | 40.411 | 59.560 | | 30.92 | |
| | 376 | CB | | | | | | | | | | AAAA |
| ATOM | | | ILE . | | 47 | | 7.144 | 39.024 | 60.167 | | 31.22 | AAAA |
| ATOM | 377 | | ILE . | | 47 | 48 | 3.093 | 37.97C | 59.640 | | 28.55 | AAAA |
| ATOM | 378 | CG1 | ILE . | A | 47 | 47 | 7.220 | 39.063 | 61.694 | 1.00 | 32.04 | AAAA |
| ATOM | 379 | CD1 | ILE . | A | 47 | 48 | 3.596 | 39.241 | 62.242 | | 34.13 | AAAA |
| ATOM | 380 | C | ILE A | | 47 | | 7.138 | 40.381 | 58.076 | | | |
| | | | | | | | | | | | 29.70 | AAAA |
| ATOM | 381 | 0 | ILE A | | 47 | | 5.956 | 40.373 | 57.714 | | 28.42 | AAAA |
| ATOM | 382 | N | LYS 2 | 4 | 48 | 48 | 3.150 | 40.380 | 57.221 | 1.00 | 28.78 | AAAA |
| ATOM | 383 | CA | LYS A | ١. | 48 | . 47 | .920 | 40.349 | 55.784 | 1.00 | 28.42 | AAAA |
| ATOM | 384 | CB | LYS 2 | | 48 | | .203 | 40.727 | 55.055 | | 27.53 | |
| | | | | | | | | | | | | AAAA |
| MOTA | 385 | CG | LYS A | 3 | 48 | | 1.116 | 40.695 | 53.556 | 1.00 | 28.97 | AAAA |
| ATOM | 386 | CD | LYS A | A. | 48 | 50 | .464 | 41.104 | 52.941 | 1.00 | 29.67 | AAAA |
| MOTA | 387 | CE | LYS 3 | | 48 | 50 | .493 | 40.893 | 51.432 | | 29.41 | AAAA |
| | 388 | | LYS A | | 48 | | .409 | 41.645 | 50.764 | | 29.68 | |
| ATOM | | ~ | 1 V C - | • | | | | | | | | AAAA |
| ATOM | 389 | | LYS ? | | 48 | | .449 | 38.950 | 55.375 | | 27.81 | AAAA |
| ATOM | 390 | 0 | LYS F | 7 | 48 | 48 | .024 | 37.938 | 55.787 | 1.00 | 27.96 | AAAA |
| ATOM | 391 | | SER A | | 49 | | .385 | 38.892 | 54.581 | | 26.82 | AAAA |
| | 392 | | SER A | | 49 | | .854 | 37.611 | 54.141 | | 26.41 | |
| ATOM | | | | | | | | | | | | AAAA |
| ATOM | 393 | | SER A | | 49 | | .514 | 37.795 | 53.420 | | 25.40 | AAAA |
| ATOM | 394 | | SER A | | | 43 | .541 | 38.349 | 54.276 | 1.00 | 25.58 | AAAA |
| ATOM | 395 | С | SER A | | 49 | 46 | .814 | 36.891 | 53.207 | 1.00 | 26.03 | AAAA |
| ATOM | 396 | | SER A | | 49 | | .462 | 37.513 | 52.373 | | 26.98 | AAAA |
| A1011 | | - | ' | - | | | | ٠,٠٠٠ | | 4.00 | -0.50 | |
| | | • | | | | | | | | | | • |

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Figure 19-7

| MOTA | 397 | N | AR | G A | 50 | | 46.910 | 35.576 | 53.354 | 1.00 25.51 | AAAA |
|------|------------|-----|-------|-----|-----|---|--------|--------|--------|-------------------------|--------|
| ATOM | 398 | CA | AR | G A | 50 | | 47.755 | 34.794 | 52.474 | 1.00 25.45 | AAAA |
| ATOM | 399 | CB | AR | G A | 50 | | 48.807 | 33.985 | | 1.00 25.85 | AAAA |
| ATOM | 400 | | | 3 A | - | | 48.229 | 32.819 | , . – | 1.00 27.16 | AAAA |
| ATOM | 401 | | | | | | 49.280 | 31.995 | | 1.00 27.57 | |
| | | | | | | | | | | | AAAA |
| MOTA | 402 | | | | | | 48.673 | 30.896 | | 1.00 27.90 | AAAA |
| ATOM | 403 | | | 3 A | | | 48.106 | 29.820 | | 1.00 28.34 | AAAA |
| MOTA | 404 | | 1 ARC | | | | 48.055 | 29.672 | | 1.00 28.19 | AAAA |
| ATOM | 405 | NH | 2 AR | 3 A | 50 | | 47.592 | 28.884 | 55.735 | 1.00 28.62 | AAAA |
| MOTA | 406 | С | ARG | 3 A | 50 | | 46.806 | 33.834 | | 1.00 24.91 | AAAA |
| ATOM | 407 | | ARC | | | | 45.740 | 33.510 | | 1.00 23.57 | AAAA |
| ATOM | 408 | N | PRO | | | | 47.172 | 33.392 | | 1.00 24.28 | AAAA |
| ATOM | 409 | | | | 51 | | 48.361 | 33.761 | 49.770 | 1.00 24.28 | |
| | 410 | CA | | | | | | | | | AAAA. |
| MOTA | | | | | | | 46.355 | | 49.776 | 1.00 24.18 | AAAA |
| MOTA | 411 | CB | | | | | 47.012 | 32.512 | 48.390 | 1.00 24.24 | AAAA |
| ATOM | 412 | CG | | | | | 47.766 | 33.862 | 48.405 | 1.00 24.11 | AAAA |
| MOTA | 413 | С | PRO | | 51 | | 46.473 | 31.070 | 50.393 | 1.00 23.69 | AAAA |
| ATOM | 414 | 0 | PRO |) A | 51 | | 47.545 | 30.680 | 50.839 | 1.00 24.13 | AAAA |
| ATOM | 415 | N | ALA | A | 52 | | 45.381 | 30.325 | 50.422 | 1.00 23.36 | AAAA |
| ATOM | 416 | CA | ALA | A | 52 | | 45.419 | 28.972 | 50.952 | 1.00 23.64 | AAAA |
| ATOM | 417 | CB | ALA | | 52 | | 44.012 | 28.405 | | 1.00 23.86 | AAAA |
| ATOM | 418 | C. | | | 52 | | 46.260 | 28.145 | 49.994 | 1.00 23.58 | |
| ATOM | 419 | ŏ | ALA | | 52 | • | 46.240 | 28.383 | 48.806 | 1.00 24.52 | AAAA |
| | | | | | | | | | | | AAAA |
| MOTA | 420 | N | THR | | 53 | | 47.009 | 27.185 | 50.501 | 1.00 24.41 | AAAA |
| ATOM | 421 | CA | THR | | 53 | | 47.815 | 26.352 | 49.628 | 1.00 26.26 | AAAA |
| MOTA | 422 | CB | THR | | 53 | | 48.933 | 25.642 | 50.405 | 1.00 26.37 | AAAA |
| MOTA | 423 | OG: | l THR | . A | 53 | | 48.355 | 24.763 | 51.375 | 1.00 26.51 | AAAA |
| MOTA | 424 | CG2 | 2 THR | A | 53 | | 49.810 | 26.648 | 51.106 | 1.00 24.48 | AAAA |
| MOTA | 425 | С | THR | A | 53 | | 46.889 | 25.299 | 49.034 | 1.00 27.63 | AAAA |
| ATOM | 426 | 0 | THR | Α | 53 | | 45.870 | 24.982 | 49.620 | 1.00 29.22 | AAAA |
| ATOM | 427 | N | LYS | A | 54 | | 47.240 | 24.776 | 47.867 | 1.00 29.31 | AAAA |
| ATOM | 428 | CA | LYS | | 54 | | 46.450 | 23.752 | 47.189 | 1.00 30.61 | AAAA |
| ATOM | 429 | СВ | LYS | | 54 | | 47.249 | 23.182 | 46.015 | 1.00 31.68 | AAAA |
| ATOM | 430 | CG | LYS | | 54. | | 46.585 | 22:020 | 45.304 | 1.00 34.38 | AAAA |
| ATOM | 431 | CD | LYS | | 54 | | 45.449 | 22.464 | 44.417 | 1.00 36.00 | AAAA |
| ATOM | 432 | CE | LYS | | 54 | | 45.943 | 22.850 | 43.025 | 1.00 37.55 | |
| | 433 | NZ | LYS | | 54 | | 46.425 | 21.664 | 42.236 | | AAAA |
| ATOM | | | LYS | | 54 | | | | | 1.00 37.57 | AAAA |
| MOTA | 434 | C | | | | | 46.127 | 22.640 | 48.170 | 1.00 31.26 | AAAA |
| ATOM | 435 | 0 | LYS | | 54 | | 45.025 | 22.097 | 48.176 | 1.00 31.72 | AAAA |
| MOTA | 436 | N | GLU | | 55 | | 47.102 | 22.312 | 49.006 | 1.00 31.88 | AAAA |
| ATOM | 437 | CA | GLU | | 55 | | 46.961 | 21.260 | 50.011 | 1.00 32.29 | AAAA |
| ATOM | 438 | CB | GLU | | 55 | | 48.266 | 21.089 | 50.778 | 1.00 34.43 | AAAA |
| MOTA | 439 | CG | GLU | | 55 | | 48.265 | 19.901 | 51.706 | 1.00 38.39 | AAAA |
| MOTA | 440 | CD | GLU | A | 55 | | 49.513 | 19.839 | 52.584 | 1.00 41.46 | AAAA |
| ATOM | 441 | OE1 | GLU | A | 55 | | 49.745 | 18.770 | 53.200 | 1.00 43.30 | · AAAA |
| MOTA | 442 | OE2 | GLU | Α | 55 | | 50.245 | 20.859 | 52.672 | 1.00 42.45 | AAAA |
| ATOM | 443 | С | GLU | Α | 55 | | 45.851 | 21.555 | 51.013 | 1.00 30.43 | AAAA |
| ATOM | 444 | 0 | GLU | | 55 | | 45.048 | 20.681 | 51.332 | 1.00 30.59 | AAAA |
| ATOM | 445 | N | GLU | | 56 | | 45.822 | 22.782 | 51.517 | 1.00 28.23 | AAAA |
| | 446 | CA | GLU | | 56 | | 44.812 | 23.164 | 52.488 | 1.00 27.69 | |
| ATOM | | | GLU | | | | | | | | AAAA |
| ATOM | 447 | CB | | | 56 | | 45.078 | | 52.989 | 1.00 27.90 | AAAA |
| MOTA | 448 | CG | GLU | | 56 | | 46.434 | 24.721 | 53.670 | 1.00 26.64 | AAAA |
| ATOM | 449 | CD | GLU | | 56 | | 46.769 | 26.135 | 54.098 | 1.00 26.35 | AAAA |
| ATOM | 450 | OE1 | GLU | A | 56 | | 46.615 | 27.057 | 53.265 | 1.00 25.12 | AAAA |
| ATOM | 451 | OE2 | GLU | Α | 56 | | 47.213 | 26.315 | 55.255 | 1.00 25.70 | AAAA |
| ATOM | 452 | C | GLU | A | 56 | | 43.408 | 23.043 | 51.914 | 1.00 26.99 [.] | AAAA |
| ATOM | 453 | 0 | GLU | A | 56 | | 42.495 | 22.574 | 52.588 | 1.00 26.25 | AAAA |
| ATOM | 454 | N | LEU | | 57 | | 43.252 | 23.447 | 50.659 | 1.00 27.26 | AAAA |
| ATOM | 455 | CA | LEU | | 57 | | 41.965 | 23.389 | 49.967 | 1.00 27.17 | AAAA |
| | 456 | CB | LEU | | 57 | | 42.077 | 24.063 | 48.596 | 1.00 26.62 | AAAA |
| ATOM | | | | | 57 | | 42.491 | 25.545 | 48.656 | 1.00 27.64 | AAAA |
| MOTA | 457 459 | CG | LEU | | | | | | | | |
| ATOM | 458 | | LEU | | 57 | | 42.770 | 26.108 | 47.269 | 1.00 26.66 | AAAA |
| ATOM | 159 | | LEU | | 57 | | 41.389 | 26.341 | 49.349 | 1.00 26.92 | AAAA |
| ATOM | 460 | C | LEU | | 57 | | 41.552 | 21.946 | 49.796 | 1.00 27.26 | AAAA |
| ATOM | 461 | 0 | LEU | | 57 | | 40.363 | 21.612 | 49.816 | 1.00 27.53 | AAAA |
| MOTA | 462 | N | LEU | A | 58 | | 42.547 | 21.085 | 49.641 | 1.00 27.42 | AAAA |
| | | | | | | | | | | | |

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Figure 19-8

| ATOM | 463 | CA | LEU | JA | 58 | | 42.293 | 19.675 | 49.457 | 1.00 | 26.10 | AAAA |
|--------------|------------|----------|-------|-----|----------|----|------------------|------------------|------------------|------|----------------|--------------|
| MOTA | 464 | CB | LEU | JA | 58 | 4, | 43.486 | 19.019 | 48.794 | 1.00 | 25.43 | AAAA |
| ATOM | 465 | CG | LEU | JA | 58 | | 43.623 | 19.577 | 47.385 | | 26.66 | AAAA |
| ATOM | 466 | | LEU | | 58 | | 44.760 | 18.884 | 46.705 | | 27.12 | AAAA |
| ATOM | 467 | CD2 | FEG. | JA | 58 | | 42.334 | 19.355 | 46.600 | | 26.43 | AAAA |
| ATOM | 468 | С | LEU | J A | 58 | | 41.938 | 18.956 | 50.731 | | 25.79 | AAAA |
| ATOM | 469 | 0 | LEU | I A | 58 | | 41.648 | 17.763 | 50.692 | | 26.50 | AAAA |
| ATOM | 470 | N | LEU | I A | 59 | | 41.977 | 19.666 | 51.858 | | 24.91 | AAAA |
| ATOM | 471 | CA | LEU | A | 59 | | 41.595 | 19.070 | 53.136 | | 25.15 | AAAA |
| ATOM | 472 | CB | LEU | | 59 | | 41.958 | 19.991 | 54.322 | | 25.44 | AAAA |
| ATOM | 473 | CG | LEU | Α | 59 | | 43.423 | 20.280 | 54.710 | | 24.67 | AAAA |
| ATOM | 474 | CD1 | LEU | | 59 | | 43.502 | 21.461 | 55.652 | | 23.70 | AAAA |
| MOTA | 475 | CD2 | LEU | Α | 59 | | 44.044 | 19.044 | 55.357 | | 24.08 | AAAA |
| ATOM | 476 | С | LEU | Α | 59 | | 40.074 | 18.870 | 53.090 | | 25.41 | AAAA |
| ATOM | 477 | 0 | LEU | Α | 59 | | 39.503 | 18.266 | 53.993 | | 25.88 | AAAA |
| ATOM | 478 | N | PHE | Α | 60 | | 39.436 | 19.392 | 52.031 | | 25.05 | AAAA |
| ATOM | 479 | CA | PHE | Α | 60 | | 37.983 | 19.276 | 51.823 | | 24.11 | AAAA |
| ATOM | 480 | CB | PHE | Α | 60 | | 37.250 | 20.476 | 52.440 | | 21.80 | . AAAA |
| ATOM | 481 | CG | PHE | | 60 | | 35.778 | 20.534 | 52.098 | | 20.07 | AAAA |
| ATOM | 482 | CD1 | PHE | A | 60 | | 34.917 | | 52.462 | | 19.27 | AAAA |
| MOTA | 483 | CD2 | PHE | A | 60 | | 35.249 | | 51.399 | | 19.82 | AAAA |
| ATOM | 484 | CE1 | PHE | Α | 60 | | 33.550 | 19.557 | 52.136 | | 19.26 | AAAA |
| ATOM | 485 | CE2 | PHE | A | 60 | | 33.890 | 21.688 | 51.071 | | 17.45 | AAAA |
| ATOM | 486 | CZ | PHE | Α | 60 | | 33.042 | 20.652 | 51.440 | | 17.92 | AAAA |
| ATOM | 487 | С | PHE | Α | 60 | | 37.557 | 19.139 | 50.345 | 1.00 | 24.02 | AAAA |
| ATOM | 488 | 0 | PHE | A | 60 | | 36.846 | 18.201 | 49.974 | | 23.27 | AAAA |
| MOTA | 489 | N | HIS | Α | 61 | | 37.982 | 20.079 | 49.511 | 1.00 | 24.40 | AAAA |
| MOTA | 490 | CA | HIS | A | 61 | | 37.626 | 20.053 | 48.099 | 1.00 | 25.04 | AAAA |
| MOTA | 491 | CB | HIS | Α | 61 | | 37.768 | 21.449 | 47.494 | 1.00 | 24.19 | AAAA |
| MOTA | 492 | CG | HIS | A | 61 | | 36.744 | 22.429 | 47.979 | 1.00 | 24.44 | AAAA |
| MOTA | 493 | CD2 | HIS | A | 61 | | 35.429 | 22.559 | 47.683 | 1.00 | 24.12 | AAAA |
| MOTA | 494 | | HIS | | 61 | | 37.038 | 23.444 | 48.864 | 1.00 | 24.36 | AAAA |
| ATOM | 495 | | HIS | | 61 | | 35.952 | 24.159 | | 1.00 | 23.18 | AAAA |
| MOTA | 496 | | HIS | | 61 | | 34.962 | 23.643 | 48.385 | 1.00 | 23.91 | AAAA |
| ATOM | 497 | С | HIS | | 61 | | 38.416 | 19.054 | 47.253 | | 25.60 | AAAA |
| MOTA | 498 | 0 | HIS | | 61 | | 39.596 | 18.805 | 47.498 | | 26.94 | AAAA |
| MOTA | 499 | N | THR | | 62 | | 37.754 | 18.496 | 46.244 | | 26.68 | AAAA |
| ATOM | 500 | CA | THR | | 62 | | 38.369 | 17.522 | 45.333 | | 28.17 | AAAA |
| ATOM | 501 | CB | THR | | 62 | | 37.290 | 16.695 | 44.614 | | 28.15 | AAAA |
| ATOM | 502 | | THR | | 62 、 | ٠. | 36.544 | 17.541 | 43.731 | | 28.10 | AAAA |
| ATOM | 503 | | THR | | 62 | | 36.334 | 16.094 | 45.629 | | 28.24 | AAAA |
| MOTA | 504 | C | THR | | 62 | · | 39.226 | 18.217 | 44.278 | | 29.28 | AAAA |
| MOTA | 505 | 0 | THR | | 62 | | 38.876 | 19.286 | 43.792 | | 29.52 | AAAA |
| ATOM | 506 507 | N | GLU | | 63 | | 40.344 41.249 | 17.606 | 43.912 | | 31.33 | AAAA |
| ATOM | 508 | CA | GLU | | 63 | | | 18.202 | 42.928 42.536 | 1.00 | 32.42 | AAAA |
| ATOM | 509 | CB CG | GLU | | 63 63 | | 42.333 43.304 | 17.219 16.869 | 43.609 | 1 00 | 34.37 37.20 | AAAA |
| ATOM ATOM | 510 | CD | GLU | | 63 | | 44.427 | 16.022 | 43.052 | | 38.79 | AAAA |
| ATOM | 511 | | GLU | | 63 | | 45.100 | 16.499 | 42.097 | | 37.96 | AAAA |
| ATOM | 512 | | GLU | - | 63 | | 44.619 | 14.892 | 43.564 | | 39.68 | AAAA |
| ATOM | 513 | C | GLU | | 63 | | 40.607 | 18.687 | 41.639 | | 31.96 | AAAA AAAA |
| ATOM | 514 | | GLU | | 63 | | 40.824 | 19.816 | 41.215 | 1.00 | | AAAA |
| ATOM | 515 | | ASP | | 64 | | 39.845 | 17.814 | 40.998 | | 31.52 | AAAA |
| ATOM | 516 | | ASP | | 64 | | 39.204 | 18.165 | 39.753 | | 31.36 | AAAA |
| ATOM | 517 | | ASP . | | 64 | | 38.301 | 17.018 | 39.295 | | 33.99 | AAAA |
| ATOM | 518 | | ASP | | 64 | | 37.213 | 16.694 | 40.302 | | 37.38 | AAAA |
| ATOM | 519 | | ASP . | | 64 | | 36.375 | 15.801 | 40.027 | | 39.80 | AAAA |
| MOTA | 520 | OD2 | | | 64 | | 37.188 | 17.332 | 41.374 | | 38.67 | AAAA |
| ATOM | 521 | | ASP . | | 64 | | 38.412 | 19.465 | 39.902 | | 30.02 | AAAA |
| ATOM | 522 | | ASP | | 64 | | 38.462 | 20.331 | 39.026 | | 30.47 | AAAA |
| ATOM | 523 | | TYR . | | 65 | | 37.695 | 19.608 | 41.012 | | 27.51 | AAAA |
| ATOM | 524 | | TYR | | 65 | | 36.918 | 20.814 | 41.248 | 1.00 | | AAAA |
| ATOM | 525 | | TYR | | 65 | | 36.010 | 20.654 | 42.467 | | 25.42 | AAAA |
| ATOM | 526. | | TYR | | 65 | | 35.339 | 21.946 | 42.866 | | 24.90 | AAAA |
| ATOM | 527 | CD1 | | | 65 | | 34.525 | 22.636 | 41.964 | | 25.04 | AAAA |
| MOTA | 528 | CE1 | | | 65 | | 33.914 | 23.823 | 42.308 | 1.00 | | AAAA. |

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Figure 19-9

| | 500 | | | | |
|-------|-------------------|----------|---------------------------|------------|------|
| MOTA | 529 CD2 TYR A 65 | 35.525 | 22.486 44.136 | 1.00 24.65 | AAAA |
| MOTA | 530 CE2 TYR A 65 | 34.920 | 23.677 44.497 | 1.00 25.86 | AAAA |
| MOTA | 531 CZ TYR A 65 | 34.110 | 24.349 43.576 | | AAAA |
| ATOM | 532 OH TYR A 65 | 33.499 | | | |
| | | | | | AAAA |
| MOTA | 533 C TYR A 65 | 37.814 | | | AAAA |
| MOTA | 534 O TYR A 65 | 37.460 | 23.129 41.096 | 1.00 25.62 | AAAA |
| MOTA | 535 N ILE A 66 | 38.965 | 21.812 42.080 | 1.00 23.20 | AAAA |
| ATOM | 536 CA ILE A 66 | 39.877 | | | |
| | | | | | AAAA |
| MOTA | | 40.924 | | | AAAA |
| ATOM | 538 CG2 ILE A 66 | 41.927 | 23.652 43.617 | 1.00 20.00 | AAAA |
| MOTA | 539 CG1 ILE A 66 | - 40.220 | 22.289 44.729 | 1.00 20.16 | AAAA |
| ATOM | 540 CD1 ILE A 66 | 39.528 | 23.523 45.228 | | AAAA |
| ATOM | 541 C ILE A 66 | 40.558 | 23.261 41.023 | | |
| | | | | | AAAA |
| MOTA | | 40.636 | 24.425 40.665 | | AAAA |
| MOTA | 543 N ASNA 67 | 41.036 | 22.262 40.295 | | AAAA |
| ATOM | 544 CA ASN A 67 | 41.698 | 22.545 39.02 9 | 1.00 23.92 | AAAA |
| ATOM | 545 CB ASN A 67 | . 42.292 | 21.261 38.395 | | AAAA |
| MOTA | 546 CG ASN A 67 | 43.344 | 20.588 39.289 | | |
| | 547 OD1 ASN A 67 | | | | AAAA |
| MOTA | | 44.196 | 21.256 39.859 | 1.00 23.47 | AAAA |
| MOTA | 548 ND2 ASN A 67 | 43.290 | 19.258 39.392 | 1.00 23.20 | AAAA |
| MOTA | 549 C ASN A 67 | 40.717 | 23.216 38.063 | 1.00 23.82 | AAAA |
| MOTA | 550 O ASN A 67 | 41.123 | 23.996 37.204 | 1.00 24.63 | AAAA |
| ATOM | 551 N THR A 68 | 39.427 | 22.928 38.213 | 1.00 24.08 | AAAA |
| ATOM | 552 CA THR A 68 | 38.428 | 23.534 37.343 | · · | |
| | | | | 1.00 25.28 | AAAA |
| ATOM | 553 CB THR A 68 | 37.030 | 22.904 37.525 | 1.00 24.55 | AAAA |
| ATOM | 554 OG1 THR A 68 | 37.090 | 21.500 37.258 | 1.00 24.64 | AAAA |
| ATOM | 555 CG2 THR A 68 | 36.049 | 23.534 36.564 | 1.00 23.58 | AAAA |
| ATOM | 556 C THR A 68 | 38.322 | 25.023 37.664 | 1.00 26,31 | AAAA |
| ATOM | 557 O THR A 68 | 38.114 | 25.854 36.771 | 1.00 26.69 | AAAA |
| ATOM | 558 N LEU A 69 | 38.462 | 25.351 38.945 | 1.00 26.59 | |
| | 559 CA LEU A 69 | | | | AAAA |
| ATOM | | 38.381 | 26.729 39.378 | 1.00 27.05 | AAAA |
| ATOM | 560 CB LEU A 69 | 38.321 | 26.807 40.904 | 1.00 27.15 | AAAA |
| MOTA | 561 CG LEU A 69 | 37.003 | 26.397 41.551 | 1.00 25.68 | AAAA |
| MOTA | 562 CD1 LEU A 69 | 37.088 | 26.491 43.062 | 1.00 26.30 | AAAA |
| ATOM | 563 CD2 LEU A 69 | 35.933 | 27.316 41.044 | 1.00 26.14 | AAAA |
| ATOM | 564 C LEU A 69 | 39.570 | 27.508 38.867 | 1.00 28.44 | AAAA |
| ATOM | 565 O LEUA 69 | 39.425 | 28.619 38.356 | 1.00 28.59 | AAAA |
| ATOM | 566 N MET A 70 | 40.748 | 26.914 39.009 | 1.00 29.31 | |
| | 567 CA MET A 70 | 41.981 | 27.536 38.571 | | AAAA |
| MOTA | | | | 1.00 29.89 | AAAA |
| MOTA | 568 CB MET A 70 | 43.160 | 26.692 39.044 | 1.00 31.04 | AAAA |
| ATOM | 569 CG MET A 70 | 43.164 | 26.528 40.562 | 1.00 31.79 | AAAA |
| MOTA | 570 SD MET A 70 | 44.608 | 25.684 41.183 | 1.00 32.58 | AAAA |
| ATOM | 571 CE MET A 70 | 45.859 | 26.820 40.670 | 1.00 30.82 | AAAA |
| ATOM | 572 C MET A 70 | 42.017 | 27.723 37.057 | 1.00 30.36 | AAAA |
| ATOM | 573 O MET A 70 | 42.462 | 28.769 36.559 | 1.00 30.18 | AAAA |
| MOTA | . 574 -N GLU A 71 | 41.538 | 26.719 36.328 | 1.00 30.34 | AAAA |
| | 575 CA GLU A 71 | | | | |
| ATOM | | 41.519 | | 1.00 30.73 | AAAA |
| ATOM | 576 CB GLU A 71 | 41.140 | 25.442 34.266 | 1.00 33.47 | AAAA |
| ATOM | 577 CG GLU A 71 | 41.122 | 25.430 32.731 | 1.00 37.11 | AAAA |
| ATOM | 578 CD GLU A 71 | 42.513 | 25.676 32.093 | 1.00 40.49 | AAAA |
| ATOM | 579 OE1 GLU A 71 | 42.570 | 25.798 30.844 | 1.00 41.95 | AAAA |
| ATOM | 580 OE2 GLU A 71 | 43.541 | 25.738 32.825 | 1.00 40.74 | AAAA |
| ATOM | 581 C GLU A 71 | 40.537 | 27.851 34.392 | 1.00 29.78 | AAAA |
| | 582 O GLU A 71 | 40.852 | 28.642 33.508 | 1.00 27.82 | |
| MOTA | | | | | AAAA |
| MOTA | 583 N ALA A 72 | 39.352 | 27.855 34.992 | 1.00 29.85 | AAAA |
| ATOM | 584 CA ALA A 72 | 38.296 | 28.790 34.635 | 1.00 29.88 | AAAA |
| MOTA | 585 CB ALA A 72 | 37.022 | 28.432 35.374 | 1.00 29.07 | AAAA |
| ATOM | 586 C ALA A 72 | 38.667 | 30.238 34.907 | 1.00 30.78 | AAAA |
| ATOM | 587 O ALA A 72 | 38.359 | 31.122 34.108 | 1.00 31.27 | AAAA |
| | 588 N GLU A 73 | 39.336 | 30.491 36.023 | 1.00 31.07 | |
| ATOM | | | | | AAAA |
| ATOM | 589 CA GLU A 73 | 39.710 | 31.856 36.346 | 1.00 31.65 | AAAA |
| MOTA | 590 CB GLU A 73 | 40.243 | 31.954 37.785 | 1.00 30.52 | AAAA |
| ATOM | 591 CG GLU A 73 | 40.643 | 33.370 38.198 | 1.00 28.73 | AAAA |
| MOTA | 592 CD GLU A 73 | 41.076 | 33.484 39.651 | 1.00 28.77 | AAAA |
| ATOM | 593 OE1 GLU A 73 | 40.239 | 33.260 40.546 | 1.00 28.94 | AAAA |
| ATOM | 594 OE2 GLU A 73 | 42.258 | 33.795 39.906 | 1.00 28.57 | AAAA |
| ALUM. | 222 000 000 11 | | | | www |

| ATOM | 595 | С | GLU A | 73 | 40.726 | 32.461 | 35.378 | 1.00 33.54 | AAAA |
|-------|------------|-----|--------|------------|----------|--------|--------|------------|--------|
| ATOM | 596 | Q | GLU A | | 40.456 | 33.499 | 34.767 | 1.00 34.93 | AAAA |
| ATOM | 597 | N | ARG A | | 41.885 | 31.832 | 35.214 | 1.00 34.35 | AAAA |
| ATOM | 598 | ĊА | ARG A | _ | 42.890 | 32.428 | 34.334 | 1.00 36.04 | AAAA |
| ATOM | 599 | CB | ARG A | | 44.238 | 31.710 | 34.482 | 1.00 36.92 | AAAA |
| ATOM- | 600 | CG | ARG A | | 44.327 | 30.313 | 33.923 | 1.00 38.14 | AAAA |
| | 601 | CD | ARG A | | 45.508 | 29.589 | 34.543 | 1.00 39.55 | AAAA |
| ATOM | 602 | NE | ARG A | | 45.893 | 28.404 | 33.785 | 1.00 42.02 | AAAA |
| ATOM | | CZ | ARG A | | 46.632 | 28.436 | 32.675 | 1.00 42.69 | AAAA |
| ATOM | 603 | | -ARG A | | 47.071 | 29.593 | 32.191 | 1.00 42.76 | AAAA |
| ATOM | 604 | | | | 46.933 | 27.309 | 32.046 | 1.00 42.70 | AAAA |
| MOTA | 605 | | ARG A | | 42.476 | 32.532 | 32.864 | 1.00 42.92 | AAAA |
| MOTA | 606 | Ç | ARG A | | | 33.493 | 32.187 | 1.00 37.73 | AAAA |
| MOTA | 607 | 0 | ARG A | | 42.842 | 31.567 | 32.367 | | |
| ATOM | 608 | N | SER A | | 41.711 | | 30.987 | 1.00 36.60 | AAAA |
| ATOM | 609 | CA | SER A | | 41.248 | 31.622 | | 1.00 36.82 | AAAA |
| MOTA | 610 | СВ | SER A | | 40.916 | 30.218 | 30.478 | 1.00 36.10 | - AAAA |
| ATOM | 611 | OG | SER A | | 39.736 | 29.723 | 31.083 | 1.00 36.39 | AAAA |
| MOTA | 612 | С | SER A | | 39.980 | 32.476 | 31.001 | 1.00 36.90 | AAAA |
| ATOM | 613 | 0 | SER A | | 39.401 | 32.791 | 29.963 | 1.00 36.25 | AAAA |
| ATOM | 614 | N | GLN A | | 39.568 | 32.845 | 32.208 | 1.00 37.62 | AAAA |
| ATOM | 615 | CA | GLN A | 76 | 38.368 | 33.639 | 32.427 | 1.00 37.92 | AAAA |
| MOTA | 616 | CB | GLN A | 76 | 38.613 | 35.100 | 32.049 | 1.00 38.23 | AAAA |
| ATOM | 617 | CG | GLN A | | 37.630 | 36.048 | 32.717 | 1.00 40.67 | AAAA |
| MOTA | 618 | CD | GLN A | . 76 | 37.929 | 36.298 | 34.199 | 1.00 41.40 | AAAA |
| ATOM | 619 | OE1 | GLN A | .76 | 38.226 | 35.379 | 34.973 | 1.00 40.79 | AAAA |
| ATOM | 620 | NE2 | GLN A | 76 | 37.833 | 37.556 | 34.597 | 1.00 42.32 | AAAA |
| ATOM | 621 | С | ĠŁN A | 76 | 37.223 | 33.064 | 31.600 | 1.00 37.75 | AAAA |
| ATOM | 622 | 0 | GLN A | 76 | . 36.521 | 33.789 | 30.901 | 1.00 38.13 | AAAA |
| ATOM | 623 | N | SER A | .77 | 37.045 | 31.749 | 31.685 | 1.00 37.52 | AAAA |
| ATOM | 624 | CA | SER A | 77 | 35.990 | 31.061 | 30.950 | 1.00 37.75 | AAAA |
| ATOM | 625 | CB | SER A | 77 | 36.537 | 30.440 | 29.664 | 1.00 37.90 | · AAAA |
| ATOM | 626 | OG | SER A | 77 | 36.851 | 31.441 | 28.724 | 1.00 40.32 | AAAA |
| ATOM | 627 | С | SER A | 77 | 35.338 | 29.960 | 31.757 | 1.00 37.55 | AAAA |
| ATOM | 628 | 0 | SER A | 7 7 | 35.790 | 29.620 | 32.846 | 1.00 35.81 | AAAA |
| ATOM | 629 | N | VAL A | 78 | 34.264 | 29.412 | 31.198 | 1.00 37.82 | AAAA |
| ATOM | 630 | CA | VAL A | 78 | 33.538 | 28.309 | 31.812 | 1.00 37.99 | AAAA |
| MOTA | 631 | CB | VAL A | 78 | 32.027 | 28.514 | 31.715 | 1.00 37.19 | AAAA |
| ATOM | 632 | CG1 | VAL A | 78 | 31.310 | 27.439 | 32.497 | 1.00 36.84 | AAAA |
| ATOM | 633 | CG2 | VAL A | 78 | 31.662 | 29.906 | 32.201 | 1.00 37.60 | AAAA |
| ATOM | 634 | С | VAL A | 78 | 33.918 | 27.089 | 30.976 | 1.00 38.28 | AAAA |
| ATOM | 635 | 0 | VAL A | 78 | 33.497 | 26.959 | 29.819 | 1.00 39.18 | AAAA |
| ATOM | 636 | N | PRO A | 79 | 34.734 | 26.187 | 31.537 | 1.00 37.69 | AAAA |
| ATOM | 637 | CD | PRO A | 79 | 35.347 | 26.167 | 32.869 | 1.00 37.65 | AAAA |
| ATOM | 638 | CA | PRO A | 79 | 35.146 | 24.998 | 30.797 | 1.00 37.54 | AAAA |
| ATOM | 639 | CB | PRO A | 79 | 36.127 | 24.325 | 31.759 | 1.00 37.45 | AAAA |
| ATOM | 640 | CG | PRO A | 79 | 36.655 | 25.489 | 32.557 | 1.00 37.65 | AAAA |
| ATOM | 641 | С | PRO A | 79 | 33.980 | 24.089 | 30.434 | 1.00 37.20 | AAAA |
| ATOM | 642 | 0 | PRO A | 79 | 32.958 | 24.050 | 31.120 | 1.00 36.43 | AAAA |
| ATOM | 643 | N | LYS A | 80 | 34.154 | 23.363 | 29.338 | 1.00 37.42 | AAAA |
| ATOM | 644 | CA | LYS A | 80 | 33.160 | 22.423 | 28.855 | 1.00 37.35 | AAAA |
| ATOM | 645 | CB | LYS A | 80 | 33.757 | 21.586 | 27.725 | 1.00 37.99 | AAAA |
| ATOM | 646 | CG | LYS A | 80 | 32.928 | 20.379 | 27.280 | 1.00 38.94 | AAAA |
| ATOM | 647 | CD | LYS A | 80 | 31.835 | 20.710 | 26.286 | 1.00 39.07 | AAAA |
| ATOM | .648 | CE | LYS A | 80 | 31.320 | 19.402 | 25.688 | 1.00 40.43 | AAAA |
| ATOM | 649 | NZ | LYS A | 80 | 30.498 | 19.543 | 24.450 | 1.00 40.48 | AAAA |
| MOTA | 650 | С | LYS A | 80 | 32.752 | 21.515 | 30.003 | 1.00 36.85 | AAAA |
| ATOM | 651 | 0 | LYS A | 80 | 33.610 | 20.942 | 30.676 | 1.00 36.56 | AAAA |
| ATOM | 652 | N | GLY A | 81 | 31.443 | 21.408 | 30.217 | 1.00 35.94 | AAAA |
| ATOM | 653 | CA | GLY A | 81 | 30.903 | 20.570 | 31.268 | 1.00 35.48 | AAAA |
| ATOM | 654 | C | GLY A | 81 | 31.110 | 21.054 | 32.693 | 1.00 35.23 | AAAA |
| | 655 | o | GLY A | 81 | 30.749 | 20.355 | 33.644 | 1.00 35.46 | AAAA |
| FIOM | 656 | N | ALA A | 82 | 31.677 | 22.241 | 32.867 | 1.00 35.17 | AAAA |
| ATOM | | CA | ALA A | 82 | 31.919 | 22.743 | 34.213 | 1.00 35.02 | AAAA |
| ATOM | 657 658 | CB | ALA A | 82 | 33.076 | 23.743 | 34.208 | 1.00 35.13 | AAAA |
| ATOM | 659 | C. | ALA A | 82 | 30.674 | 23.378 | 34.797 | 1.00 34.39 | AAAA |
| ATOM | 660 | 0 | ALA A | 82 | 30.451 | 23.332 | 36.001 | 1.00 33.82 | AAAA |
| ATOM | 000 | • | Water | | 20.434 | | - | | • |

; **226/263** Figure 19-11

| ATOM | 661 | N | ARG | Α | 83 | 29.858 | 3 1 23,960 | 33.932 | 1.00 34.77 | AAAA |
|--------|------|-----|-------|------|------------|---------|------------|--------|------------|--------|
| ATOM | 662 | | ARG | | 83 | 28.637 | | | | |
| | 663 | | | | | | | | | AAAA |
| ATOM | | | ARG | | 83 | 27.899 | - | | | AAAA |
| ATOM | 664 | CG | ARG | Α | 83 | 27.045 | 26.395 | 33.464 | 1.00 37.09 | AAAA |
| ATOM | 665 | CD | ARG | Α | 83 | 26,209 | 26.141 | 34.686 | 1.00 37.48 | AAAA |
| ATOM | 666 | NE | ARG | Α | 83 | 25.475 | 27.310 | 35.134 | 1.00 37.35 | AAAA |
| ATOM | 667 | CZ | ARG | | 83 | 24.711 | | | 1.00 37.77 | |
| | 668 | | | | | | | | | AAAA |
| ATOM | | | L ARG | | 83 | 24.606 | | | | AAAA |
| ATOM | 669 | | 2 ARG | | 83 | 24.040 | | 36.568 | 1.00 38.34 | AAAA |
| ATOM | 670 | С | ARG | A | 83 | 27.739 | 23.603 | 35.065 | 1.00 36.30 | AAAA |
| MOTA | 671 | 0 | ARG | Α | 83 | 27.232 | 23.854 | 36.154 | 1.00 36.17 | AAAA |
| ATOM | 672 | N | GLU | | 84 | 27.565 | | | 1.00 37.19 | |
| | 673 | | | | _ | | | | | AAAA |
| ATOM | | CA | GLU | | 84 | 26.721 | | | 1.00 37.80 | AAAA |
| MOTA | 674 | CB | GLU | A. | 84 | 26.466 | 20.375 | 33.833 | 1.00 40.55 | AAAA |
| ATOM | 675 | CG | GLU | Α | 84 | 25.643 | 19.171 | 34.232 | 1.00 43.12 | AAAA |
| MOTA | 676 | CD | GLU | Α | 84 | 25.362 | 18.268 | 33.046 | 1.00 44.98 | AAAA |
| ATOM | 677 | | GLU | | 84 | 24.573 | | | 1.00 46.36 | |
| | 678 | | GLU | | | | - | | | AAAA |
| ATOM | | | | | 84 | 25.937 | | | 1.00 44.94 | AAAA |
| `ATOM | 679 | С | GLU | | 84 | 27.290 | | | 1.00 37.07 | AAAA |
| ATOM | 680 | 0 | GLU | A | 84 | 26.642 | 20.555 | 37.199 | 1.00 36.17 | AAAA |
| ATOM | 681 | N | LYS | Α | 85 | 28.506 | 20.152 | 35.999 | 1.00 36,23 | AAAA |
| ATOM | 682 | CA | LYS | | 85 | 29,202 | | | 1.00 35.36 | |
| | 683 | | LYS | | 85 | | | | | AAAA |
| ATOM | | CB | | | | 30.449 | | | 1.00 36.96 | AAAA |
| MOTA | 684 | CG | LYS | | 85 | 31.394 | | | 1.00 39.04 | AAAA |
| MOTA | 685 | CD | LYS | A | 85 | 30.995 | 16.766 | 37.919 | 1.00 40.59 | AAAA |
| MOTA | 686 | CE | LYS | Α | 85 | 31.508 | 15.719 | 36.933 | 1.00 41.88 | AAAA |
| ATOM | 687 | NZ | LYS | A | 85 | 32.998 | 15.817 | 36.757 | 1.00 42.00 | AAAA |
| ATOM | 688 | C | LYS | | 85 | 29.620 | 20.202 | 38.289 | 1.00 33.86 | |
| | | | | | | | | | | AAAA |
| ATOM | 689 | 0 | LYS | | 85 | 29.576 | 19.679 | 39.404 | 1.00 33.82 | AAAA |
| ATOM | 690 | N | TYR | | 86 | 30.014 | 21.458 | 38.097 | 1.00 32.06 | AAAA |
| MOTA | 691 | CA | TYR | A | 86 | 30.514 | 22.279 | 39.194 | 1.00 29.44 | AAAA |
| ATOM | 692 | CB | TYR | Α | 86 | 31.956 | 22.683 | 38.875 | 1.00 29.97 | AAAA |
| MOTA | 693 | CG | TYR | Α | 86 | 32.872 | 21.496 | 38.621 | 1.00 29.99 | AAAA |
| ATOM | 694 | CD1 | | | 86 ' | 33.281 | 20:666 | 39.666 | 1.00 29.24 | |
| | 695 | | | | | | | | | AAAA |
| ATOM . | | CE1 | | | 86 | 34.126 | 19.582 | 39.437 | 1.00 29.85 | AAAA |
| ATOM | 696 | CD2 | TYR | | 86 | .33.329 | 21.204 | 37.329 | 1.00 30.16 | AAAA |
| MOTA | 697 | CE2 | TYR . | A | 86 | 34.173 | 20.118 | 37.087 | 1.00 29.61 | AAAA |
| MOTA | 698 | CZ | TYR . | A | 86 . | 34.570 | 19.313 | 38.148 | 1.00 29.79 | AAAA |
| ATOM | 699 | ОН | TYR . | A | 86 | 35.414 | 18.253 | 37.923 | 1.00 29.48 | AAAA |
| MOTA | 700 | C | TYR | | 86 | 29.705 | 23.509 | 39.572 | 1.00 27.81 | AAAA |
| | 701 | | | | | | | | | |
| MOTA | | 0 | TYR . | | 86 | 30.052 | 24.202 | 40.524 | 1.00 27.56 | AAAA |
| ATOM | 702 | Ŋ | ASN . | | 87 | 28.642 | 23.784 | 38.828 | 1.00 26.60 | AAAA |
| ATOM | 703 | CA | ASN A | A. I | 87 | 27.777 | 24.924 | 39.111 | 1.00 26.56 | AAAA |
| ATOM | 704 | CB | ASN A | A' 8 | 87 | 27.172 | 24.772 | 40.508 | 1.00 26.39 | AAAA |
| ATOM | 705 | CG | ASN 2 | A 1 | 87 | 25.863 | 25.544 | 40.684 | 1.00 26.64 | AAAA |
| MOTA | 706 | | ASN A | | 87. | 25.335 | 25.632 | 41.790 | 1.00 26.84 | |
| | | | | | | | | | | AAAA |
| ATOM | 707 | | ASN A | | 37 | 25.330 | 26.084 | 39.597 | 1.00 26.33 | AAAA |
| ATOM | 708 | С | ASN A | A 8 | 37 | 28.587 | 26.217 | 39.024 | 1.00 26.40 | AAAA |
| MOTA | 709 | 0 | ASN A | A 8 | 3 7 | 28.430 | 27.129 | 39.832 | 1.00 24.80 | AAAA |
| ATOM | 710 | N | ILE A | ٤ ۾ | 88 | 29.448 | . 26.273 | 38.015 | 1.00 27.57 | AAAA |
| ATOM | 711 | CA | ILE A | | 38 | 30.330 | 27.409 | 37.767 | 1.00 27.88 | |
| | | | | | | | | | | AAAA |
| ATOM | 712 | | ILE A | | 88 | 31.817 | 26.932 | 37.648 | 1.00 27.38 | AAAA |
| MOTA | 713 | CG2 | ILE A | 7 8 | 38 | 32.684 | 27.994 | 36.986 | 1.00 26.34 | AAAA |
| ATOM | 714 | CG1 | ILE A | A 8 | 88 | 32.354 | 26.543 | 39.026 | 1.00 28.35 | AAAA |
| ATOM | 715 | | ILE A | | 18 | 32.356 | 27.671 | 40.042 | 1.00 27.78 | AAAA |
| ATOM | 716 | | ILE A | | 18 | 29.946 | 28.110 | 36.472 | 1.00 29.17 | |
| | | | | | | 20.240 | | | | AAAA |
| ATOM | 717 | | ILE A | | 8 | 29.530 | 27.469 | 35.515 | 1.00 29.75 | AAAA |
| MOTA | 718 | | GLY A | | 19 | 30.092 | 29.429 | 36.443 | 1.00 29.96 | AAAA |
| ATOM | 719 | CA | GLY A | 8 | 9 | 29.791 | 30.162 | 35.229 | 1.00 30.24 | AAAA |
| ATOM | 720 | | GLY A | | 9. | 28.430 | 30.805 | 35.242 | 1.00 30.44 | AAAA |
| ATOM | 721 | | GLY A | | 9 | 28.177 | 31.769 | 34.514 | 1.00 31.14 | AAAA |
| | | | | | | | | | | |
| MOTA | 722 | | GLY A | _ | 0 | 27.542 | 30.268 | 36.061 | 1.00 30.00 | AAAA . |
| ATOM | 723 | | GLY A | | 0 | 26.221 | 30.841 | 36.129 | 1.00 30.52 | AAAA |
| ATOM | 724 | C (| GLY A | . 9 | 0 | 26.283 | 32.262 | 36.661 | 1.00 31.09 | AAAA |
| ATOM | 725 | | GLY A | _ | 0 | 27.356 | 32.795 | 36.962 | 1.00 30.34 | AAAA |
| | 726 | | TYR A | | i | 25.112 | 32.873 | 36.768 | 1.00 31.09 | AAAA |
| ATOM | . 20 | 7.A | TIV W | . , | • | 2J.112 | 26.013 | | 1.00 31.03 | ann |

| ATOM | 727 | CA | TYI | R A | 91 | 24.977 | 34.213 | 37.290 | 1.00 31.27 | AAAA |
|------|-------|-----|-----|-----|----|----------|--------|--------|------------|------|
| ATOM | 728 | CB | TYI | R A | 91 | 23.515 | 34.634 | 37.195 | 1.00 31.82 | AAAA |
| ATOM | 729 | CG | | R A | | 23.169 | 35.825 | 38.047 | 1.00 31.81 | AAAA |
| ATOM | 730 | | TY | | | 23.536 | 37.108 | 37.670 | 1.00 32.44 | AAAA |
| ATOM | 731 | | TY | | | 23.250 | 38.203 | 38.475 | | |
| | | | | | | | | | 1.00 31.88 | AAAA |
| ATOM | 732 | CD2 | | | 91 | 22.505 | 35.663 | 39.254 | 1.00 32.63 | AAAA |
| ATOM | 733 | CE2 | | | 91 | 22.215 | 36.754 | 40.068 | 1.00 32.60 | AAAA |
| MOTA | 734 | CZ | TYF | | 91 | 22.589 | 38.016 | 39.668 | 1.00 31.59 | AAAA |
| ATOM | 735 | ОН | TYF | łΑ | 91 | 22.283 | 39.094 | 40.450 | 1.00 31.94 | AAAA |
| ATOM | 736 | С | TYF | λ | 91 | 25.384 | 34.202 | 38.753 | 1.00 31.56 | AAAA |
| MOTA | 737 | 0 | TYF | A | 91 | 26.075 | 35.105 | 39.233 | 1.00 31.21 | AAAA |
| ATOM | 738 | N | GLU | JΑ | 92 | 24.925 | 33.158 | 39.438 | 1.00 31.51 | AAAA |
| ATOM | 739 | CA | GLU | JΑ | 92 | 25.143 | 32.941 | 40.865 | 1.00 32.70 | AAAA |
| MOTA | 740 | CB | GLU | JA | 92 | 24.463 | 31.626 | 41.268 | 1.00 33.55 | AAAA |
| ATOM | 741 | CG | GLU | | 92 | 24.174 | 31.495 | 42.747 | 1.00 34.16 | AAAA |
| ATOM | 742 | CD | GLU | | 92 | 23.311 | 30.278 | 43.087 | 1.00 35.31 | AAAA |
| ATOM | 743 | | GLU | | 92 | 23.857 | 29.148 | 43.152 | 1.00 34.30 | |
| | 744 | OE2 | | | 92 | 22.076 | | 43.275 | | AAAA |
| ATOM | | | | | | | 30.466 | | 1.00 35.36 | AAAA |
| MOTA | 745 | C | GLU | | 92 | 26.619 | 32.902 | 41.248 | 1.00 33.02 | AAAA |
| ATOM | 746 | 0 | GLU | | 92 | 27.073 | 33.623 | 42.140 | 1.00 32.91 | AAAA |
| MOTA | 747 | Ŋ | ASN | | 93 | 27.358 | 32.049 | 40.550 | 1.00 32.84 | AAAA |
| MOTA | 748 | CA | ASN | | 93 | 28.785 | 31.861 | 40.777 | 1.00 31.92 | AAAA |
| ATOM | 749 | CB | ASN | Α | 93 | 29.015 | 30.437 | 41.278 | 1.00 31.18 | AAAA |
| ATOM | 750 | CG | ASN | Α | 93 | 27.948 | 29.994 | 42.259 | 1.00 30.34 | AAAA |
| ATOM | 751 | OD1 | ASN | A | 93 | 27.723 | 30.642 | 43.271 | 1.00 31.20 | AAAA |
| ATOM | 752 | ND2 | ASN | Α | 93 | 27.284 | 28.892 | 41.955 | 1.00 29.02 | AAAA |
| ATOM | 753 | С | ASN | A | 93 | 29.442 | 32.052 | 39.411 | 1.00 30.84 | AAAA |
| MOTA | 754 | Ö | ASN | | 93 | 29.823 | 31.082 | 38.758 | 1.00 30.82 | AAAA |
| ATOM | 755 | N | PRO | | 94 | 29.605 | 33.309 | 38.975 | 1.00 29.56 | AAAA |
| MOTA | 756 | CD | PRO | | 94 | 29.312 | 34.590 | 39.626 | 1.00 29.03 | AAAA |
| MOTA | 757 | CA | PRO | | 94 | 30.209 | 33.564 | 37.671 | 1.00 28.89 | AAAA |
| | 758 | CB | PRO | | 94 | 29.890 | 35.045 | 37.416 | 1.00 28.22 | |
| MOTA | 759 | CG | PRO | | 94 | 28.839 | | 38.435 | | AAAA |
| ATOM | | | | | | | 35.377 | | 1.00 29.50 | AAAA |
| MOTA | . 760 | C | PRO | | | . 31.698 | 33.351 | 37.664 | 1.00 28.25 | AAAA |
| ATOM | 761 | O | PRO | | 94 | 32.308 | 32.996 | 38.671 | 1.00 28.21 | AAAA |
| MOTA | 762 | Ŋ | VAL | | 95 | 32.257 | 33.593 | 36.488 | 1.00 27.36 | AAAA |
| MOTA | 763 | CA | VAL | | 95 | 33.676 | 33.530 | 36.247 | 1.00 26.24 | AAAA |
| MOTA | 764 | CB | VAL | | 95 | 33.945 | 33.289 | 34.741 | 1.00 26.10 | AAAA |
| MOTA | 765 | CG1 | VAL | Α | 95 | 35.373 | 33.717 | 34.357 | 1.00 25.47 | AAAA |
| ATOM | 766 | CG2 | VAL | Α | 95 | 33.736 | 31.826 | 34.434 | 1.00 25.59 | AAAA |
| ATOM | 767 | С | VAL | A | 95 | 34.178 | 34.919 | 36.647 | 1.00 26.56 | AAAA |
| ATOM | 768 | 0 | VAL | Α | 95 | 33.560 | 35.937 | 36.307 | 1.00 27.18 | AAAA |
| ATOM | 769 | N | SER | A | 96 | 35.280 | 34.966 | 37.382 | 1.00 25.23 | AAAA |
| ATOM | 770 | CA | SER | A | 96 | 35.858 | 36.237 | 37.790 | 1.00 24.51 | AAAA |
| ATOM | 771 | СЗ | SER | | 96 | 34.935 | 36.961 | 38.774 | 1.00 23.22 | AAAA |
| ATOM | 772 | OG | SER | | 96 | 34.941 | 36.297 | 40.014 | 1.00 19.76 | AAAA |
| | 773 | c | SER | | 96 | 37.169 | 35.920 | 38.485 | 1.00 24.84 | AAAA |
| ATOM | 774 | 0 | SER | | 96 | | 34.764 | 38.530 | | |
| ATOM | | | | | | 37.590 | | | 1.00 25.97 | AAAA |
| ATOM | 775 | N | TYR | | 97 | 37.824 | 36.933 | 39.030 | 1.00 24.02 | AAAA |
| ATOM | 776 | CA | TYR | | 97 | 39.047 | 36.664 | 39.744 | 1.00 24.55 | AAAA |
| MOTA | 777 | CB | TYR | | 97 | 40.071 | 37.762 | 39.504 | 2.00 20.04 | AAAA |
| ATOM | 778 | CG | TYR | | 97 | 40.682 | 37.636 | 38.128 | 1.00 23.72 | AAAA |
| ATOM | 779 | CD1 | TYR | A. | 97 | 40.177 | 38.341 | 37.039 | 1.00 23.11 | AAAA |
| ATOM | 780 | CE1 | TYR | A | 97 | 40.700 | 38.136 | 35.758 | 1.00 23.50 | AAAA |
| MOTA | 781 | CD2 | TYR | A | 97 | 41.717 | 36.735 | 37.903 | 1.00 22.25 | AAAA |
| ATOM | 782 | CE2 | TYR | A | 97 | 42.236 | 36.526 | 36.640 | 1.00 22.86 | AAAA |
| ATOM | 783 | CZ | TYR | | 97 | 41.730 | 37.217 | 35.572 | 1.00 23.56 | AAAA |
| ATOM | 784 | OH | TYR | | 97 | 42.232 | 36.941 | 34.318 | 1.00 24.06 | AAAA |
| | 785 | C | TYR | | 97 | 38.800 | 36.436 | 41.228 | 1.00 25.08 | AAAA |
| MOTA | | | TYR | | 97 | 39.739 | 36.266 | 42.009 | 1.00 25.08 | AAAA |
| ATOM | 786 | 0 | | | | 37.522 | | 41.589 | | |
| ATOM | 787 | N | ALA | | 98 | | 36.406 | | 1.00 24.73 | AAAA |
| ATOM | 788 | CA | ALA | | 98 | 37.083 | 36.159 | 42.951 | 1.00 24.50 | AAAA |
| MOTA | 789 | CB | ALA | | 98 | 35.800 | 36.925 | 43.235 | 1.00 24.48 | AAAA |
| ATOM | 790 | C | ALA | | 98 | 36.824 | 34.661 | 43.088 | 1.00 23.95 | AAAA |
| ATOM | 791 | Ο. | ALA | | 98 | 36.929 | 34.100 | 44.171 | 1.00 24.21 | AAAA |
| ATCM | 792 | N | MET | A | 99 | 36.502 | 34.011 | 41.976 | 1.00 23.10 | AAAA |
| • | | | | | | | | - | | |

| ATOM | 793 CA MET A 99 | 36.208 | 32.584 | 42.000 | 1.00 22.61 | AAAA |
|-------|-------------------|----------|--------|--------|------------|------|
| ATOM | 794 CB MET A 99 | 35.855 | | | | |
| ATOM | 795 CG MET A 99 | 37.009 | | | | AAAA |
| ATOM | | | | | | AAAA |
| | | 36.360 | | | | AAAA |
| ATOM | 797 CE MET A 99 | 35.328 | | 38.258 | 1.00 22.04 | AAAA |
| MOTA | 798 C MET A 99 | 37.319 | 31.720 | 42.581 | 1.00 21.80 | AAAA |
| MOTA | 799 O MET A 99 | 37.052 | | | | AAAA |
| ATOM | 800 N PHE A 100 | 38.567 | | | | |
| ATOM | 801 CA PHE A 100 | | | | 1.00 21.87 | AAAA |
| | | 39.650 | | | | AAAA |
| ATOM | 802 CB PHE A 100 | 40.388 | | 41.841 | 1.00 20.25 | AAAA |
| ATOM | 803 CG PHE A 100 | 41.451 | 29.648 | 42.375 | 1.00 20.14 | AAAA |
| ATOM | 804 CD1 PHE A 100 | 41.114 | 28.462 | 43.010 | | AAAA |
| ATOM | 805 CD2 PHE A 100 | 42.785 | | | 1.00 19.82 | • |
| MOTA | 806 CE1 PHE A 100 | 42.090 | | | | AAAA |
| ATOM | 807 CE2 PHE A 100 | | | | 1.00 19.54 | AAAA |
| | | 43.755 | | | 1.00 19.22 | AAAA |
| ATOM | 808 CZ PHE A 100 | 43.410 | 28.122 | | 1.00 19.47 | AAAA |
| MOTA | 809 C PHE A 100 | 40.649 | 32.161 | 43.743 | 1.00 21.37 | AAAA |
| MOTA | 810 O PHE A 100 | 40.959 | 31.822 | 44.887 | 1.00 21.26 | AAAA |
| ATOM | 811 N THR A 101 | 41.142 | 33.252 | | 1.00 20.94 | |
| ATOM | 812 CA THR A 101 | 42.119 | 34.097 | | | AAAA |
| ATOM | | | | | 1.00 21.95 | AAAA |
| | | 42.691 | 35.181 | | 1.00 22.21 | AAAA |
| MOTA. | 814 OG1 THR A 101 | 43.511 | 34.552 | 41.917 | 1.00 22.90 | AAAA |
| ATOM | 815 CG2 THR A 101 | 43.535 | 36.186 | 43.667 | 1.00 21.38 | AAAA |
| ATOM | 816 C THR A 101 | 41.584 | 34.755 | 45.117 | 1.00 22.60 | AAAA |
| ATOM | 817 O THR A 101 | 42.248 | 34.723 | | 1.00 23.38 | |
| ATOM | 818 N GLY A 102 | 40.394 | 35.343 | | | AAAA |
| ATOM | | | | | 1.00 22.13 | AAAA |
| | | 39.826 | 35.972 | 46.227 | 1.00 22.03 | AAAA |
| ATOM | 820 C GLY A 102 | 39.340 | 34.928 | 47.221 | 1.00 21.36 | AAAA |
| ATOM | 821 O GLY A 102 | 39.433 | 35.104 | 48.439 | 1.00 20.02 | AAAA |
| MOTA | 822 N SER A 103 | 38.816 | 33.833 | 46.677 | 1.00 21.86 | AAAA |
| MOTA | 823 CA SER A 103 | 38.311 | 32.719 | 47.466 | 1.00 21.68 | AAAA |
| ATOM | 824 CB SER A 103 | 37.699 | 31.668 | 46.557 | 1.00 21.56 | |
| ATOM | 825 OG SER A 103 | 36.604 | 32.216 | 45.857 | | AAAA |
| ATOM | 826 C SER A 103 | | | | 1.00 23.67 | AAAA |
| | | 39.450 | 32.098 | 48.229 | 1.00 22.67 | AAAA |
| ATOM | 827 O SER A 103 | 39.314 | 31.806 | 49.412 | 1.00 22.44 | AAAA |
| MOTA | 828 N SER A 104 | 40.578 | 31.898 | 47.545 | 1.00 23.37 | AAAA |
| ATOM | 829 CA SER A 104 | 41.746 | 31.305 | 48.183 | 1.00 23.50 | AAAA |
| ATOM | 830 CB SER A 104 | 42.862 | 31.070 | 47.172 | 1.00 24.80 | AAAA |
| ATOM | 831 OG SER A 104 | 42.441 | 30.169 | 46.175 | 1.00 28.38 | AAAA |
| ATOM | 832 C SER A 104 | 42.254 | 32.230 | 49.256 | 1.00 22.79 | |
| ATOM | 833 O SER A 104 | 42.707 | | | | AAAA |
| | | | 31.794 | 50.307 | 1.00 22.66 | AAAA |
| ATOM | | 42.160 | 33.518 | 48.970 | 1.00 22.08 | AAAA |
| MOTA | 835 CA LEU A 105 | 42.626 | 34.541 | 49.870 | 1.00 21.70 | AAAA |
| ATOM | 836 CB LEU A 105 | 42.524 | 35.882 | 49.159 | 1.00 21.89 | AAAA |
| MOTA | 837 CG LEU A 105 | · 43.332 | 37.038 | 49.718 | 1.00 23.64 | AAAA |
| ATOM | 838 CD1 LEU A 105 | 44.830 | 36.692 | 49.639 | 1.00 22.01 | AAAA |
| ATOM | 839 CD2 LEU A 105 | 43.004 | | 48.919 | 1.00 23.60 | |
| ATOM | 840 C LEU A 105 | 41.767 | | | | AAAA |
| | | | 34.525 | 51.131 | 1.00 22.29 | AAAA |
| MOTA | 841 O LEU A 105 | 42.277 | 34.595 | 52.249 | 1.00 21.95 | AAAA |
| ATOM | 842 N ALA A 106 | 40.458 | 34.429 | 50.934 | 1.00 22.23 | AAAA |
| ATOM | 843 CA ALA A 106 | 39.515 | 34.394 | 52.042 | 1.00 22.32 | AAAA |
| MOTA | 844 CB ALA A 106 | 38.068 | 34.472 | 51.526 | 1.00 22.05 | AAAA |
| ATOM | 845 C ALA A 106 | 39.704 | 33.126 | 52.840 | 1.00 21.99 | |
| ATOM | 846 O ALA A 106 | | | | | AAAA |
| | | 39.578 | 33.145 | 54.061 | 1.00 23.18 | AAAA |
| ATOM | 847 N THR A 107 | 40.011 | 32.032 | 52.144 | 1.00 21.24 | AAAA |
| MOTA | 848 CA THR A 107 | 40.209 | 30.732 | 52.779 | 1.00 20.60 | AAAA |
| ATOM | 849 CB THR A 107 | 40.170 | 29.571 | 51.749 | 1.00 19.82 | AAAA |
| MOTA | 850 CG1 THR A 107 | 38.903 | 29.553 | 51.083 | 1.00 18.56 | AAAA |
| ATOM | 851 CG2 THR A 107 | 40.360 | 28.242 | 52.455 | 1.00 18.58 | |
| | | | | | | AAAA |
| ATOM | 852 C THR A 107. | 41.516 | 30.630 | 53.561 | 1.00 21.41 | AAAA |
| ATOM | 953 O THR A 107 | 41.537 | 30.040 | 54.646 | 1.00 23.16 | AAAA |
| ATOM | 854 N GLY A 108 | 42.601 | 31.176 | 53.003 | 1.00 20.14 | AAAA |
| ATOM | 855 CA GLY A 108 | 43.878 | 31.145 | 53.684 | 1.00 18.20 | AAAA |
| ATOM. | 856 C GLY A 108 | 43.739 | 31.933 | 54.972 | 1.00 18.43 | AAAA |
| ATOM | 857 O GLY A 108 | 44.335 | _ | | | |
| | | | 31.600 | 55.998 | 1.00 17.52 | AAAA |
| ATOM | 858 N SER A 109 | 42.909 | 32.969 | 54.929 | 1.00 18.56 | AAAA |

| MOTA | 859 | CA | SER . | A 109 | 42.683 | 33.805 | 56.098 | 1.00 19.67 | AAAA |
|--------------|------|-----|---------|---------|--------|--------|----------------|------------|--------------|
| | 860 | CB | | A 109 | 41.899 | 35.058 | 55.707 | 1.00 20.27 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 861 | OG | | A 109 | 42.618 | 35.803 | 54.746 | 1.00 21.80 | AAAA |
| ATOM | 862 | С | SER . | A 109 | 41.955 | 33.066 | 57.219 | 1.00 19.61 | AAAA |
| • | 863 | O | SER | A 109 | 42.078 | 33.426 | 58.388 | 1.00 18.40 | AAAA |
| ATOM | | | | | | | | 1.00 19.88 | |
| ATOM - | 864 | N | THR | A 110 | 41.186 | 32.042 | 56.866 | | AAAA |
| MOTA | 865 | CA | THR . | A 110 | 40.493 | 31.288 | 57.891 | 1.00 20.51 | AAAA |
| | | | | | 39.365 | 30.438 | 57.304 | 1.00 20.62 | ÄAAA |
| MOTA | 866 | CB | | A 110 | | | | | |
| ATOM | 867 | 0G1 | THR . | A 110 | 38.236 | 31.284 | 57.050 | 1.00 20.80 | AAAA |
| ATOM | 868 | CG2 | THR | A 110 | 38.974 | 29.313 | 58.262 | 1.00 20.53 | AAAA |
| | | | | | | 30.420 | 58.601 | 1.00 20.36 | AAAA |
| MOTA | 869 | С | • | A 110 | 41.504 | | | | |
| ATOM | 870 | 0 | THR . | A -110 | 41.455 | 30.268 | 59.822 | 1.00 20.78 | AAAA |
| | 871 | N | VAT. | A 111 . | 42.431 | 29.855 | 57.832 | 1.00 20.85 | AAAA |
| ATOM | | | | | | | 58.423 | 1.00 21.03 | AAAA |
| MOTA | 872 | CA | | A 111 | 43.480 | 29.053 | | | |
| MOTA | 873 | CB | VAL . | A 111 | 44.318 | 28.323 | 57.345 | 1.00 21.05 | AAAA |
| | 874 | CGI | 17AT. | A 111 | 45.537 | 27.644 | 57.983 | 1.00 19.91 | -AAAA |
| MOTA | | | | | | | 56.648 | 1.00 18.39 | AAAA |
| MOTA | 875 | CGZ | VAL | A 111 | 43.460 | 27.281 | | | |
| ATOM | 876 | С | VAL A | A 111 | 44.374 | 30.005 | 59.232 | 1.00 21.84 | AAAA |
| | 877 | 0 | | A 111 | 44.825 | 29.671 | 60.331 | 1.00 22.73 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 878 | N | GLN A | A 112 | 44.612 | 31.204 | 58.712 . | | AAAA |
| MOTA | 879 | CA | GLN A | A 112 | 45.449 | 32.133 | 59.452 | 1.00 21.89 | AAAA |
| | 880 | CB | | A 112 | 45.630 | 33.450 | 58.690 | 1.00 22.50 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 881 | CG | GLN A | A 112 | 46.288 | 33.283 | 57.335 | 1.00 23.68 | AAAA |
| ATOM | 882 | CD | GLN A | A 112 | 46.414 | 34.578 | 56.569 | 1.00 23.18 | AAAA |
| | | | GLN A | | 47.389 | 35.310 | 56.722 | 1.00 23.86 | AAAA |
| MOTA | 883 | | | _ | | | | | |
| ATOM | 884 | NE2 | GLN A | A 112 | 45.413 | 34.879 | 55.752 | 1.00 21.90 | AAAA |
| ATCM | 885 | С | GLN A | A 112 | 44.766 | 32.383 | 60.774 | 1.00 21.84 | AAAA |
| | 886 | 0 | | A 112 | 45.389 | 32.316 | 61.835 | 1.00 22.47 | AAAA |
| ATOM | | | | | | | 60.700 | 1.00 21.34 | AAAA |
| MOTA | 887 | N | | A 113 | 43.468 | 32.651 | | | |
| ATOM | 888 | CA | ALA A | A 113 | 42.682 | 32.934 | 61.884 | 1.00 20.84 | AAAA |
| | 889 | CB | | A 113 | 41.244 | 33.172 | 61.504 | 1.00 18.52 | AAAA |
| ATOM | | | | | | | 62.865 | 1.00 21.75 | AAAA |
| ATOM | 890 | С | | A 113 | 42.795 | 31.782 | | | |
| ATOM | 891 | 0 | ALA A | A 113 | 42.880 | 31.985 | 64.084 | 1.00 22.24 | AAAA |
| | 892 | N | TIR | A 114 | 42.797 | 30.569 | 62.329 | 1.00 22.54 | AAAA |
| ATOM | | | | | | 29.393 | 63.160 | 1.00 23.16 | AAAA |
| MOTA | 893 | | ILE A | | 42.891 | | | • | |
| ATOM | 894 | CB | ILE A | A 114 | 42.557 | 28.146 | 62.352 | 1.00 23.33 | AAAA |
| ATOM | 895 | CG2 | ILE 2 | A 114 | 42.939 | 26.912 | 63.106 | 1.00 23.80 | AAAA |
| | | | | | 41.058 | 28.130 | 62.047 | 1.00 23.48 | AAAA |
| MOTA | 896 | | ILE A | | | | | | |
| ATOM | 897 | CD1 | ILE A | A 114 | 40.610 | 26.951 | 61.204 | 1.00 22.08 | AAAA |
| ATOM | 898 | С | TLE | A 114 | 44.268 | 29.270 | 63.792 | 1.00 24.33 | AAAA |
| | | | | A 114 | 44.373 | 29.013 | 64.990 | 1.00 25.30 | AAAA |
| ATOM | 899 | 0 | | | | | | | |
| MOTA | 900 | N | GLU A | A 115 | 45.319 | 29.490 | 63.002 | 1.00 24.96 | AAAA |
| ATOM | 901 | CA | GLU A | A 115 | 46.699 | 29.395 | 63.503 | 1.00 26.61 | AAAA |
| | | | | A 115 | 47.708 | 29.753 | 62.406 | 1.00 24.75 | AAAA |
| ATOM | 902 | CB | | | | | | | AAAA |
| ATOM | 903 | CG | GLU A | A 115 | 47.444 | 29.033 | 61.103 | 1.00 25.80 | |
| ATOM | 904 | CD | GLU A | A 115 | 48.471 | 29.323 | 60.030 | 1.00 26.07 | AAAA |
| | 905 | | GLU A | | 48.911 | 30.484 | 59.940 | 1.00 27.15 | AAAA |
| ATOM | | | | | | | | 1.00 25.45 | AAAA |
| ATOM | 906 | | GLU A | | 48.819 | 28.402 | 59.260 | | |
| ATOM | 907 | С | GLU A | A 115 | 46.877 | 30.340 | 64.680 | 1.00 27.89 | AAAA |
| | 908 | ō | | A 115 | 47.480 | 29.975 | 65.695 | 1.00 28.04 | AAAA |
| ATOM | | | | | | _ | 64.531 | 1.00 29.15 | AAAA |
| ATOM | 909 | N | | A 116 | 46.337 | 31.552 | | | |
| MOTA | 910 | CA | GLU A | A 116 | 46.408 | 32.579 | 65.563 | 1.00 29.42 | AAAA |
| | 911 | CB | CT.II 2 | A 116 | 45.751 | 33.871 | 65.082 | 1.00 28.26 | AAAA |
| ATOM | | | | | | | 63.945 | 1.00 28.93 | AAAA |
| ATOM | 912 | CG | GLU A | A 116 ' | 46.482 | 34.529 | | | |
| ATOM | 913 | CD | GLU A | A 116 | 47.902 | 34.937 | 64.318 | 1.00 28.32 | AAAA |
| | 914 | | GLU A | | 48.081 | 35.878 | 65.123 | 1.00 27.68 | AAAA |
| ATOM | | | | | | | 63.810 | 1.00 27.38 | AAAA |
| ATOM | 91,5 | OE2 | GLU 1 | | 48.838 | 34.297 | | | |
| ATOM | 916 | С | GLU A | A 116 | 45.737 | 32.126 | 66.845 | 1.00 29.77 | AAAA |
| | 917 | ō | | A 116 | 46.338 | 32.196 | 67.920 | 1.00 30.29 | AAAA |
| ATOM | | | | | | | 66.727 | 1.00 29.64 | AAAA |
| ATCM | 918 | N | PHE A | | 44.492 | 31.665 | | | |
| ATOM | 919 | CA | PHE 2 | a 117 | 43.741 | 31.204 | 67.88 7 | 1.00 29.33 | AAAA |
| | | CB | | A 117 | 42.425 | 30.552 | 67.480 | 1.00 28.89 | AAAA |
| ATOM | 920 | | | | | | 68.651 | 1.00 28.93 | AAAA |
| ATOM | 921 | CG | | A 117 | 41.604 | 30.087 | 50.001 | _ | |
| | | | DITTO 3 | 117 | 41.010 | 31.010 | 69.510 | 1.00 28.42 | AAAA |
| 2/P/OM | 922 | CDI | PRE A | 3 77/ | | | | | |
| ATOM | 922 | | PHE A | | | | 68.910 | 1.00 29.06 | AAAA |
| atom atom | 923 | CD2 | PHE A | A 117 | 41.441 | 28.723 | 68.910 | 1.00 29.06 | |
| | | CD2 | | A 117 | | | | | AAAA AAAA |

| MOTA | 925 | CE2 | .PHE A | 117 | 40.695 | 28.284 | 70.009 | 1.00 29.16 | AAAA |
|--------|-------|-----|--------|--------|--------|--------|--------|------------|--------|
| | | | | | | 29.227 | 70.862 | 1.00 29.03 | AAAA |
| ATOM | 926 | CZ | PHE A | 7 11 / | 40.103 | | | | |
| ATOM | 927 | С | PHE A | 117 | 44.545 | 30.195 | 68.671 | 1.00 29.22 | AAAA |
| | 928 | 0 | PHE A | | 44.677 | 30.315 | 69.884 | 1.00 30.29 | AAAA |
| ATOM | | | | | | _ | | | |
| ATOM | 929 | N | LEU A | 1118 | 45.066 | 29.195 | 67.965 | 1.00 29.24 | AAAA |
| ATOM | 930 | CA | LEU A | 118 | 45.864 | 28.145 | 68.576 | 1.00 29.50 | AAAA |
| | | | | | | | | | |
| MOTA | 931 | CB | LEU A | 7 778 | 46.182 | 27.047 | 67.550 | 1.00 28.57 | АААА |
| ATOM | 932 | CG | LEU A | 118 | 44.962 | 26.296 | 66.989 | 1.00 28.16 | AAAA |
| | | CD1 | LEU A | | 45.421 | 25.090 | 66.191 | 1.00 25.58 | AAAA |
| ATOM | 933 | | | | | | | | |
| ATOM | 934 | CD2 | LEU A | 118 | 44.053 | 25.846 | 68.128 | 1.00 27.64 | , AAAA |
| ATOM | 935 | С | LEU A | 118 | 47.150 | 28.649 | 69.227 | 1.00 30,14 | AAAA |
| | | | | | | | 70.056 | | |
| MOTA | 936 | 0 | LEU A | 7 778 | 47.727 | 27.954 | | 1.00 29.94 | AAAA |
| ATOM | 937 | N | LYS A | 119 | 47.602 | 29.845 | 68.847 | 1.00 31.36 | AAAA |
| | | CA | LYS A | | 48.798 | 30.451 | 69.448 | 1.00 32.52 | AAAA |
| MOTA | 938 | | | | | | | | |
| MOTA | 939 | CB | LYS A | 119 | 49.396 | 31.539 | 68.559 | 1.00 32.38 | AAAA |
| ATOM | 940 | CG | LYS A | 119 | 49.882 | 31.108 | 67.199 | 1.00 33.03 | AAAA |
| | | | | | | | | | |
| ATOM | 941 | CD | LYS A | 119 | 50.371 | 32.321 | 66.411 | 1.00 32.74 | AAAA |
| ATOM | 942 | CE | LYS A | 119 | 50.681 | 31.939 | 64.972 | 1.00 33.94 | AAAA |
| | 943 | NZ | LYS A | | 51.125 | 33:099 | 64.152 | 1.00 34.93 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 944 | С | LYS A | . 119 | 48.385 | 31.143 | 70.744 | 1.00 33.74 | AAAA |
| ATOM | 945 | 0 | LYS A | 119 | 49.218 | 31.748 | 71.413 | 1.00 34.85 | AAAA |
| | 946 | N | GLY A | | 47.096 | 31.079 | 71.073 | 1.00 33.68 | AAAA |
| MOTA | | | | | | | | | |
| MOTA | 947 | CA | GLY A | . 120 | 46.600 | 31.736 | 72.263 | 1.00 33.69 | AAAA |
| ATOM | 948 | С | GLY A | . 120 | 45.987 | 33.110 | 71.988 | 1.00 34.11 | AAAA |
| ATOM | 949 | 0 | GLY A | | 45.588 | 33.802 | 72.932 | 1.00 33.65 | AAAA |
| | | | | | | | | 1.00 33.58 | |
| MOTA | 950 | N | ASN A | | 45.904 | 33.513 | 70.717 | | AAAA |
| ATOM | 951 | CA | ASN A | . 121 | 45.326 | 34.820 | 70.368 | 1.00 33.35 | AAAA |
| ATOM | 952 | CB | ASN A | 121 | 46.194 | 35.537 | 69.341 | 1.00 33.18 | AAAA |
| | | | | | | 35.828 | 69.859 | 1.00 34.31 | AAAA |
| ATOM | 953 | CG | ASN A | | 47.570 | | | | |
| ATOM | 954 | OD1 | ASN A | . 121 | 48.333 | 34.921 | 70.154 | 1.00 35.67 | AAAA |
| MOTA | 955 | ND2 | ASN A | 121 | 47.897 | 37.096 | 69.975 | 1.00 34.18 | AAAA |
| | | | | | | 34.805 | 69.839 | 1.00 32.85 | AAAA |
| MOTA | 956 | C | ASN A | | 43.888 | | | | |
| MOTA | 957 | 0 | ASN A | 121 | 43.304 | 33.751 | 69.599 | 1.00 32.78 | AAAA |
| ATOM | 958 | N | VAL A | 122 | 43.338 | 36.003 | 69.655 | 1.00 32.47 | AAAA |
| | 959 | CA | VAL A | | 41.980 | 36.200 | 69.148 | 1.00 30.89 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 960 | CB | VAL A | 122 | 41.182 | 37.145 | 70.070 | 1.00 31.05 | AAAA |
| ATOM | 961 | CG1 | VAL A | 122 | 39.831 | 37.423 | 69.489 | 1.00 30.95 | AAAA: |
| | 962 | CG2 | VAL A | 122 | 41.038 | 36.516 | 71.440 | 1.00 31.19 | AAAA |
| MOTA | | | | | | | | 1.00 30.19 | AAAA |
| MOTA | 963 | С | VAL A | 122 | 42.056 | 36.805 | 67.750 | | |
| ATOM . | 964 | 0 | VAL A | 122 | 42.694 | 37.840 | 67.535 | 1.00 31.28 | AAAA |
| | 965 | N | ALA A | 123 | 41.405 | 36.147 | 66.800 | 1.00 28.62 | AAAA |
| ATOM | | | | | | | 65.421 | 1.00 26.49 | AAAA |
| MOTA | 966 | CA | ALA A | 123 . | 41.415 | 36.589 | | | |
| ATOM | 967 | CB | ALA A | 123 | 42.323 | 35.708 | 64.599 | 1.00 26.51 | AAAA |
| ATOM | 968 | С | ALA A | 123 | 40.038 | 36.570 | 64.836 | 1.00 25.59 | AAAA |
| | | | | | | | 65.252 | 1.00 26.27 | AAAA |
| MOTA | 969 | 0 | ALA A | | 39.173 | 35.814 | | | |
| ATOM | 970 | N | PHE A | 124 | 39.848 | 37.421 | 62.847 | 1.00 25.44 | AAAA |
| ATOM | 971 | CA | PHE A | 124 | 38.590 | 37.534 | 61.156 | 1.00 23.87 | AAAA |
| | | | | | | 38.779 | 63.646 | 1.00 23.58 | AAAA |
| ATOM | 972 | CB | PHE A | | 37.832 | | | | |
| MOTA | 973 | CG | PHE A | 124 | 36.591 | 39.119 | 62.841 | 1.00 23.71 | AAAA |
| ATOM. | 974 | CD1 | PHE A | 124 | 35.668 | 38.140 | 62.495 | 1.00 23.44 | AAAA |
| | | | | | | 40.449 | 62.498 | 1.00 23.75 | AAAA |
| MOTA | 975 | | PHE A | | 36.311 | | | | |
| ATOM | 976 | CE1 | PHE A | 124 | 34.479 | 38.483 | 61.823 | 1.00 23.31 | AAAA |
| MOTA | 977 | CE2 | PHE A | 124 | 35.131 | 40.796 | 61.833 | 1.00 21.71 | AAAA |
| | | | PHE A | | 34.217 | 39.815 | 61.497 | 1.00 22.35 | AAAA |
| ATOM | . 978 | CZ | | | | | | | |
| MOTA | 979 | С | PHE A | 124 | 38.951 | 37.673 | 61.700 | 1.00 23.26 | AAAA |
| ATOM | 980 | 0 | PHE A | 124 | 39.720 | 38.555 | 61.323 | 1.00 22.29 | AAAA |
| | | | ASN A | | 38.427 | 36.759 | 60.897 | 1.00 23.24 | AAAA |
| ATOM | 981 | N | | | | | | | |
| MOTA | 982 | CA | ASN A | 125 | 38.622 | 36.785 | 59.457 | 1.00 21.08 | AAAA |
| ATOM | 983 | СВ | ASN A | 125 | 39.181 | 35.470 | 58.951 | 1.00 19.90 | AAAA |
| | | | ASN A | | 39.098 | 35.360 | 57.454 | 1.00 20.64 | AAAA |
| ATOM | 984 | CG | M MCM | 165 | | | | | |
| MOTA | 985 | OD1 | ASN A | 125 | 39.389 | 36.317 | 56.748 | 1.00 21.63 | AAAA |
| ATOM | 986 | ND2 | ASN A | 125 | 38.721 | 34.190 | 56.956 | 1.00 19.93 | AAAA |
| | | | ASN A | 125 | 37.269 | 37.059 | 58.813 | 1.00 20.19 | AAAA |
| MOTA | 987 | C | | | | | | 1.00 19.21 | AAAA |
| ATOM | 988 | 0 | ASN A | 125 | 36.469 | 36.148 | 58.579 | | |
| ATOM | 989 | N | PRO A | 126 | 36.991 | 38.340 | 58.543 | 1.00 19.14 | AAAA |
| | | | | | | | | | |
| ATOM | 990 | CD | PRO A | 126 | 37.893 | 39.460 | 58.858 | 1.00 19.22 | AAAA |

SUBSTITUTE SHEET (RULE 26)

| ATOM | 991 | | | 126 | 35.766 | 38.849 | 57.932 | 1.00 | 19.52 | AAAA |
|--------------|--------------|----|---------|-------|------------------|------------------|------------------|------|----------------|--------|
| ATOM | 992 | | | 126 | 36.005 | 40.359 | 57.941 | | 18.55 | AAAA |
| ATOM | 993 | | | | 37.511 | 40.465 | 57.799 | 1.00 | 17.97 | AAAA |
| ATOM | 994 | | PRO A | 126 | 35.456 | 38.313 | 56.526 | 1.00 | 19.41 | AAAA |
| ATOM | 995 | | PRO A | | 34.303 | 38.349 | 56.080 | | 19.68 | AAAA |
| MOTA | 996 | | ALA A | | 36.477 | 37.814 | 55.835 | | 18.17 | AAAA |
| MOTA | 997 | | | | 36.283 | 37.314 | 54.481 | | 17.66 | AAAA |
| MOTA | 998 | | | | 37.547 | 37.520 | 53.658 | | 17.08 | AAAA |
| ATOM | 999 | | ALA A | - 127 | 35.875 | 35.857 | 54.443 | 1.00 | 17.46 | AAAA |
| ATOM | 1000 | | ALA A | 127 | 35.438 | 35.359 | 53.409 | | 18.92 | AAAA |
| ATOM | 1001 | N | GLY A | 128 | 36.019 | 35.180 | 55.570 | | 15.94 | AAAA |
| MOTA | 1002 | CA | GLY A | 128 | 35.685 | 33.780 | 55.642 | 1.00 | 15.45 | AAAA |
| MOTA | 1003 | С | GLY A | 128 | 34.226 | 33.593 | 55.955 | 1.00 | 16.08 | AAAA |
| ATOM | 1004 | 0 | GLY A | 128 | 33.485 | 34.557 | 55.997 | | 15.43 | AAAA |
| ATOM | 1005 | N | GLY A | 129 | 33.821 | 32.353 | 56.198 | 1.00 | 16.77 | AAAA |
| ATOM | 1006 | CA | GLY A | 129 | 32.426 | 32.082 | 56.462 | 1.00 | 17.82 | AAAA |
| ATOM | 1007 | C | GLY A | 129 | 31.669 | 31.822 | 55.169 | | 18.64 | AAAA |
| MOTA | 1008 | 0 | GLY A | 129 | 30.469 | 32.051 | 55.108 | | 18.48 | AAAA |
| MOTA | 1009 | N | MET A | 130 | 32.380 | 31.368 | | | 20.45 | AAAA |
| ATOM | 1010 | CA | MET A | 130 | 31.790 | 31.029 | 52.826 | | 21.60 | AAAA |
| MOTA | 1011 | CB | MET A | 130 | 32.866 | 31.117 | 51.744 | | 22.02 | AAAA |
| ATOM | 1012 | CG | MET A | 130 | 33.551 | 32.472 | 51.698 | | 21.75 | AAAA |
| ATOM | 1013 | SD | MET A | | 34.971 | 32.567 | 50.599 | | 24.75 | AAAA |
| ATOM | 1014 | CE | MET A | | 34.268 | 32.137 | 49.048 | | 24.40 | AAAA |
| ATOM | 1015 | С | MET A | | 31.328 | 29.587 | 53.002 | | 22.08 | AAAA |
| ATOM | 1016 | 0 | MET A | 130 | 31.970 | 28.641 | 52.546 | 1.00 | 22.98 | AAAA |
| MOTA | 1017 | N | HIS A | | 30.184 | 29.452 | 53.659 | | 22.25 | AAAA |
| ATOM | 1018 | CA | HIS A | | 29.618 | 28.171 | 54.062 | 1.00 | 20.49 | AAAA |
| ATOM | 1019 | CB | HIS A | | 28.832 | 28.421 | 55.342 | 1.00 | 20.00 | AAAA |
| ATOM | 1020 | CG | HIS A | | 27.679 | 29.360 | 55.161 | 1.00 | 17.93 | AAAA. |
| ATOM | 1021 | | HIS A | | 27.091 | 29.846 | 54.043 | 1.00 | 17.88 | AAAA |
| ATOM | 1022 | | HIS A | | 26.952 | 29.854 | 56.219 | | 19.33 | AAAA |
| MOTA | 1023 | | HIS A | | 25.968 | 30.607 | 55.758 | 1.00 | 16.99 | AAAA |
| ATOM | 1024 | | HIS A | | 26.031 | 30.617 | 54.441 | 1.00 | 17.43 | AAAA |
| ATOM | 1025 | C | HIS A | | 28.763 | 27.332 | 53.141 | | 19.97 | AAAA |
| MOTA | 1026 | 0 | HIS A | | 28.330 | 26.262 | 53.541 | | 19.61 | · AAAA |
| MOTA | 1027 | N | HIS A | | 28.518 | 27.796 | 51.923 | | 20.11 | AAAA |
| ATOM | 1028 | CA | HIS A | | 27.673 | 27.058 | 50.994 | | 17.76 | AAAA |
| ATOM ATOM | 1029 1030 | CB | HIS A | | 26.879 | 28.044 | 50.127 | | 16.76 | AAAA |
| ATOM | 1030 | CG | HIS A | | 25.824 | 28.815 | 50.862 | | 15.35 | AAAA |
| ATOM | 1031 | | HIS A | | 25.567 | 30.146 | 50.920 | | 14.15 | AAAA |
| ATOM | 1032 | | HIS A | | 24.804 | 28.200 | 51.557 | | 16.15 | AAAA |
| ATOM | 1034 | | HIS A | | 23.966 24.405 | 29.119 | 52.005 | | 14.13 | AAAA |
| MOTA | 1035 | C | HIS A | | 28.355 | 30.307 | 51.632 | | 14.65 | AAAA |
| ATOM | 1.36 | ō | HIS A | | 27.742 | 26.051 | 50.065 | | 17.99 | AAAA |
| ATOM | 1.37 | N | ALA A | | 29.604 | 25.053 26.305 | 49.684 49.690 | | 18.54 | - AAAA |
| ATOM | 1.38 | CA | ALA A | | 30.300 | 25.441 | 48.742 | | 17.82 | AAAA |
| ATOM | 1039 | CB | ALA A | | 31.684 | 25.961 | 48.507 | | 18.38 17.53 | AAAA |
| ATOM | 1040 | c | ALA A | | 30.366 | 23.970 | 49.130 | | | AAAA |
| ATOM | 1041 | ō | ALA A 1 | _ | 30.578 | 23.633 | 50.298 | | 20.92 | AAAA |
| ATOM | 1042 | N | PHE A | | 30.184 | 23.086 | 48.152 | | 21.79 | AAAA |
| ATOM | 1043 | CA | PHE A 1 | | 30.258 | 21.663 | 48.455 | | 20.58 | AAAA |
| ATOM | 1044 | СВ | PHE A 1 | | 29.168 | 20.860 | 47.731 | | _ | AAAA |
| ATOM | 1045 | CG | PHE A 1 | | 27.772 | 21.229 | 48.126 | | 19.41 | AAAA |
| ATOM | 1046 | | PHE A 1 | | 27.027 | | | | 18.32 | AAAA . |
| ATOM | 1047 | | PHE A 1 | | 27.193 | 22.099 | 47.357 49.271 | | 19.22 | AAAA |
| ATOM | 1048 | | PHE A 1 | | 25.714 | 20.701 | | | 19.14 | AAAA |
| ATOM | 1049 | | PHE A 1 | | 25.889 | 22.438 | 47.726 | | 18.56 | AAAA |
| ATOM | 1050 | | PHE A 1 | | 25.158 | 21.036 | 49.644 | | 17.72 | AAAA |
| ATOM | 1051 | | PHE A 1 | | | 21.903 | 48.866 48.081 | | 18.01 | AAAA |
| ATOM | 1052 | | PHE A 1 | | 32.459 | 21.124 | | • | 22.90 | AAAA |
| ATOM | 1053 | | LYS A 1 | | 31.842 | 21.833 | 47.544 48.390 | | 23.37 | AAAA |
| ATOM | 1054 | | LYS A 1 | | | 19.861 | | | 24.63 | AAAA |
| ATOM | 1054 | | LYS A 1 | | | 19.195 | 48.122 | 1.00 | 27.16 | AAAA |
| ATOM | 1056 | | LYS A 1 | | 32.926 | 17.714 | 48.480 | 1.00 | 28.53 | AAAA |
| 011 | T030 | | _+0 N T | | 34.133 | 16.843 | 48.292 | 1.00 | 31.01 | AAAA |
| | | | | | | | | | | • |

| MOTA | 1057 | CD | LYS A 135 | 33.879 | 15.472 | 48.910 | 1.00 32.75 | AAAA |
|--------------|--------------|----------|------------------------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 1058 | CE | LYS A 135 | 33.961 | 15.495 | 50.457 | 1.00 33.96 | AAAA |
| ATOM | 1059 | NZ | LYS A 135 | 35.371 | 15.664 | 50.976 | 1.00 33.04 | AAAA |
| MOTA | 1060 | С | LYS A 135 | 33.577 | 19.390 | 46.673 | 1.00 27.37 | AAAA |
| ATOM | 1061 | 0 | LYS A 135 | 34.769 | 19.596 | 46.437 | 1.00 27.35 | AAAA |
| MOTA | 1062 | N | SER A 136 | 32.658 | 19.354 | 45.714 | 1.00 27.32 | AAAA |
| MOTA | 1063 | CA | _SER A 136 | 33.028 | 19.527 | 44.313 | 1.00 28.31 | AAAA |
| MOTA | 1064 | CB | SER A 136 | 33.093 | 18.162 | 43.626 | 1.00 28.56 | AAAA |
| ATOM | 1065 | OG | SER A 136 | 33.822 | 17.242 | 44.417 | 1.00 29.28 | AAAA |
| MOTA | 1066 | С | SER A 136 | 31.993 | 20.395 | 43.599 | 1.00 28.91 | AAAA |
| MOTA | 1067 | 0 | SER A 136 | - 31.568 | 20.080 | 42.486 | 1.00 28.78 | AAAA |
| ATOM | 1068 | N | ARG A 137 | 31.595 | 21.502 | 44.212 | 1.00 29.08 | AAAA. |
| MOTA | 1069 | CA | ARG A 137 | 30.574 | 22.311 | 43.576 | 1.00 29.66 | AAAA |
| MOTA | 1070 | CB | ARG A 137 | 29.259 | 21.528 | 43.657 | 1.00 31.65 | AAAA |
| ATOM | 1071 | CG | ARG A 137 | 27.989 | 22.273 | 43.355 | 1.00 33.89 | AAAA |
| ATOM | 1072 | CD | ARG A 137 | 26.862 | 21.267 | 43.373 | 1.00 35.93 | AAAA |
| MOTA | 1073 | NE C7 | ARG A 137 | 26.961 26.505 | 20.366 | 42.228 | 1.00 36.31 | AAAA |
| ATOM | 1074 1075 | CZ | ARG A 137 ARG A 137 | 25.915 | 20.660 21.834 | 41.015 40.798 | 1.00 35.99 1.00 34.63 | AAAA |
| ATOM ATOM | 1075 | | ARG A 137 | 26.650 | 19.786 | 40.738 | 1.00 34.83 | AAAA |
| ATOM | 1077 | . C | ARG A 137 | 30.402 | 23.723 | 44.116 | 1.00 28.53 | AAAA AAAA |
| ATOM | 1078 | ō | ARG A 137 | 30.418 | 23.946 | 45.324 | 1.00 28.51 | AAAA |
| ATOM | 1079 | Ŋ | ALA A 138 | 30.247 | 24.673 | 43.202 | 1.00 27.53 | AAAA |
| ATOM: | 1080 | CA | ALA A 138 | 30.039 | 26.063 | 43.581 | 1.00 27.64 | AAAA |
| ATOM | 1081 | CB | ALA A 138 | 30.236 | 26.984 | 42.381 | 1.00 27.87 | AAAA |
| ATOM | 1082 | C | ALA A 138 | 28,601 | 26.130 | 44.079 | 1.00 27.27 | AAAA |
| ATOM | 1083 | 0 | ALA A 138 | 27.769 | 25.321 | 43.671 | 1.00 28.30 | AAAA |
| ATOM | 1084 | N | ASN A 139 | 28.292 | 27.080 | 44.951 | 1.00 26.16 | AAAA |
| ATOM | 1085 | CA | ASN A 139 | 26.945 | 27.134 | 45.480 | 1.00 25.39 | AAAA |
| ATOM | 1086 | CB | ASN A 139 | 26.673 | 25.847 | 46.282 | 1.00 24.58 | AAAA |
| MOTA | 1087 | CG | ASN A 139 | 25.343 | 25.872 | 47.017 | 1.00 25.37 | AAAA |
| ATOM | 1088 | | ASN A 139 | 24.272 | 26.017 | 46.413 | 1.00 24.20 | AAAA |
| ATOM | 1089 | | ASN A 139 | 25.408 | 25.720 | 48.338 | 1.00 24.91 | AAAA |
| ATOM | 1090 | Ċ | ASN A 139 | | 28.358 | 46.341 | 1.00 24.90 | AAAA |
| ATOM | 1091 | 0 | ASN A 139 | 27.346 | 28.570 | 47.348 | 1.00 24.98 | AAAA |
| MOTA | 1092 | N | GLY A 140 | 25.702 | 29.145 | 45.916 | 1.00 24.46 | AAAA |
| MOTA | 1093 | CA C | GLY A 140 GLY A 140 | 25.294 26.383 | 30.336 31.358 | 46.625 46.755 | 1.00 22.96 1.00 22.24 | AAAA |
| ATOM | 1094 1095 | 0 | GLY A 140 | 26.663 | 31.336 | 47.867 | 1.00 22.24 | AAAA AAAA |
| atom Atom | 1095 | N | PHE A 141 | 26.992 | 31.711 | 45.625 | 1.00 20.60 | AAAA |
| MOTA | 1097 | CA | PHE A 141 | 28.075 | 32.700 | 45.572 | 1.00 19.43 | AAAA |
| ATOM | 1098 | CB | PHE A 141 | 27.758 | 33.920 | 46.430 | 1.00 19.86 | AAAA |
| MOTA | 1099 | CG | PHE A 141 | 26.453 | 34.577 | 46.114 | 1.00 21.18 | AAAA |
| ATOM | 1100 | CD1 | PHE A 141 | 25.974 | 35.592 | 46.934 | 1.00 20.49 | AAAA |
| ATOM " | 1101 | CD2 | PHE A 141 | 25.723 | 34.218 | 44.985 | 1.00 21.42 | · AAAA |
| MOTA | 1102 | CE1 | PHE A 141 | 24.800 | 36.242 | 46.638 | 1.00 ?2.45 | AAAA |
| ATOM | 1103 | CE2 | PHE A 141 | 24.540 | 34.859 | 44.672 | 1.00 :1.76 | AAAA |
| MOTA | 1104 | CZ | PHE A 141 | 24.072 | 35.881 | 45.499 | 1.00 ~3.05 | AAAA |
| MOTA | 1105 | C | PHE A 141 | 29.396 | 32.132 | 46.069 | 1.00 18.68 | AAAA |
| ATOM | 1106 | 0 | PHE A 141 | 30.438 | | 45.944 | 1.00 19.19 | AAAA |
| MOTA | 1107 | N . | CYS A 142 | 29.367 | 30.930 | 46.635 | 1.00 16.93 | AAAA |
| MOTA | 1108 | CA | CYS A 142 | 30.594 | 30.332 | 47.150 | 1.00 16.80 | AAAA · |
| MOTA | 1109 | CB | CYS A 142 | 30.323 | 29.689 | 48.509 | 1.00 16.51 | AAAA |
| ATOM | 1110 | SG | CYS A 142 | 29.524 | 30.826 | 49.617 | 1.00 15.01 | AAAA |
| MOTA | 1111 | C | CYS A 142 CYS A 142 | 31.227 30.533 | 29.315 28.565 | 46.221 45.556 | 1.00 16.45 1.00 15.32 | AAAA |
| ATOM | 1112 | .O . | | | | | ** ** | AAAA |
| MOTA | 1113 1114 | N CA | TYR A 143 TYR A 143 | 32.558 33.340 | 29.311 28.394 | 46.190 45.362 | 1.00 18.39 1.00 18.63 | AAAA AAAA |
| MOTA | 1115 | CB | TYR A 143 | 34.298 | 29.154 | 44.438 | 1.00 18.63 | AAAA |
| ATOM | 1116 | CG | TYR A 143 | 33.664 | 30.214 | 43.571 | 1.00 19.48 | AAAA |
| ATOM | 1117 | | TYR A 143 | 33.480 | 31.510 | 44.043 | 1.00 19.33 | AAAA |
| ATOM ATOM | 1118 | | TYR A 143 | 32.856 | 32.473 | 43.261 | 1.00 21.63 | AAAA |
| ATOM | 1119 | | TYR A 143 | 33.212 | 29.910 | 42.292 | 1.00 20.14 | AAAA |
| ATOM | 1120 | | TYR A 143 | 32.588 | 30.863 | 41.507 | 1.00 20.82 | AAAA |
| ATOM | 1121 | CZ | TYR A 143 | 32.414 | 32.135 | 41.998 | 1.00 20.90 | AAAA |
| ATOM | 1122 | | TYR A 143 | 31.787 | 33.071 | 41.228 | 1.00 23.36 | AAAA |
| | | | | | | | | |

SUBSTITUTE SHEET (RULE 26)

| ATO | M 1123 | С | TYR | . A | 143 | | 34.162 | 27.490 | 46.283 | 1.00 1 | 19.06 | | AAAA |
|-------|--------|-----|---------------|-----|-----|---|--------|---------------|----------------|--------|--------|---|-------------|
| | | 0 | | | | | 34.319 | 26.289 | 46.032 | 1.00 1 | 10 40 | | AAAA |
| ATO | M 1124 | U | | | 143 | | | | | | | | |
| ATO | M 1125 | N | ILE | A | 144 | | 34.695 | 28.087 | 47.344 | 1.00 1 | 19.15 | | AAAA |
| | | | | | | | 35.490 | | | | | | |
| ATO | M 1126 | CA | باللا | A | 144 | | | | 48.315 | 1.00 1 | • | | AAAA |
| ATO | M 1127 | CB | ILE | A | 144 | | 36.952 | 27.861 | 48.355 | 1.00 1 | 19.74 | | AAAA |
| | | | | | | | | | 49.410 | 1.00 1 | | | |
| ATO | M 1128 | CG2 | | | 144 | | 37.757 | 27.088 | | | | | AAAA |
| ATO | м 1129 | CG1 | ILE | A | 144 | | 37.584 | 27.671 | 46.965 | 1.00 2 | 20.12 | | AAAA |
| | | | | | | | | | | 1.00 2 | | _ | |
| . ATO | M 1130 | CDI | ILE | A | 144 | | 39.053 | 28.072 | 46.846 | 1.00 4 | \$1.05 | | Aaaa |
| ATO | M 1131 | С | TLE | Δ | 144 | | 34.833 | 27.532 | 49.665 | 1.00 2 | 20.22 | | AAAA |
| | | | | | | | | | | | | | |
| ATO | M 1132 | 0 | LILE | Α | 144 | | 34.357 | 28.626 | 49.981 | 1.00 | 19.94 | | AAAA |
| ATO | | N | A CM | Δ | 145 | | 34.787 | 26.451 | 50.440 | 1.00 2 | 20 57 | | AAAA |
| | - | | | | | | | | | | | | |
| · ATO | M 1134 | CA | ASN | Ą | 145 | | 34.165 | 26.448 | 51.770 | 1.00 2 | 20.39 | | AAAA |
| | | CB | V GM | Δ | 145 | - | 33.450 | 25.114 | 51.990 | 1.00 | 19 39 | | AAAA |
| ATO | | | | | | | | | | | | | |
| ATO | M 1136 | CG | ASN | A | 145 | | 32.505 | 25.143 | 53.171 | 1.00 | 19.31 | | AAAA |
| | | OD1 | ASN | - λ | 145 | | 32.862 | 25.583 | 54.263 | 1.00 2 | 21 26 | | AAAA |
| ATO | | | | | | | | | | | | | |
| ATO | M 1138 | ND2 | ASN | A | 145 | | 31.290 | 24.667 | 52.960 | 1.00 | 17.08 | - | AAAA |
| | | С | | | 145 | | 35.236 | | 52.856 | 1.00 2 | 20 17 | | AAAA |
| ATO | | | | | | | | | | | | | |
| ATO | M 1140 | 0 | ASN | A | 145 | | 35.690 | 25.622 | 53.421 | 1.00 3 | 19.75 | | AAAA |
| | | N | | | 146 | | 35.644 | 27.862 | 53.148 | 1.00 2 | 20 06 | | AAAA |
| ATO | | | | | | | | | | | | | |
| ATO | M 1142 | CA | ASN | A | 146 | | 36.671 | 28.075 | 54.166 | 1.00 2 | 20.98 | | AAAA |
| | | CB | አ ሮእ ኒ | 70 | 146 | | 37.019 | 29.573 | 54.333 | 1.00 2 | 21 79 | | AAAA |
| ATO | _ | | | | | | | | | | | | |
| ATO: | M 1144 | CG | ASN | A | 146 | | 35.876 | 30.411 | 54.882 | 1.00 2 | 22.78 | | AAAA |
| | | OD3 | ASN | 7 | 115 | | 35.651 | 30.465 | 56.091 | 1.00 2 | 22 63 | | AAAA |
| ATO: | | | | | | | | | | | | | |
| ATO | M 1146 | ND2 | ASN | Α | 146 | | 35.144 | 31.078 | 53.983 | 1.00 2 | 23.70 | | AAAA |
| | | C | | | 146 | | 36.307 | 27.413 | 55.496 | 1.00 2 | 21 18 | | AAAA |
| ATO: | | | | | | | | | | | | | |
| ATO | M 1148 | 0 | ASN | А | 146 | | 37.169 | 26.823 | 56.139 | 1.00 2 | 21.48 | | AAAA |
| | | N | ספפ | ת | 147 | | 35.031 | 27.476 | 55.922 | 1.00 2 | 20.88 | | AAAA |
| ATO: | | | | | | | | | | | | | |
| ATO: | M 1150 | CD | PRO | A | 147 | | 33.835 | 28.120 | 55.358 | 1.00 2 | 21.85 | | AAAA |
| | | CA | PRO | Δ | 147 | | 34.674 | 26.831 | 57.183 | 1.00 2 | 21.42 | | AAAA |
| ATO: | | | | | | | | | | | | | |
| ATO: | M 1152 | CB | PRO | А | 147 | | 33.176 | 27.073 | 57.261 | 1.00 2 | 21.00 | | AAAA |
| | | CG | PRO | Δ | 147 | - | 33.052 | 28.408 | 56.605 | 1.00 2 | 20.47 | | AAAA |
| ATO: | | | | | | | | | | | | | |
| ATO: | M 1154 | С | PRO. | . А | 147 | | 35.015 | 25.334 | 57.174 | 1.00 2 | 22.19 | | AAAA |
| | | 0 | חממ | Δ | 147 | | 35.650 | 24.833 | 58.099 | 1.00 2 | 25.69 | | AAAA |
| ATO: | | | | | | | | • | | | | | |
| ATO | M 1156 | N | ALA | A | 148 | | 34.603 | 24:616 | 56.136 | 1.00 2 | | | AAAA |
| ATO | | CA | ALA | Δ | 148 | | 34.889 | 23.193 | 56.070 | 1.00 2 | 22.23 | | AAAA |
| | | | | | | | | | | | | | |
| ATO | M 1158 | CB | ALA | A | 148 | | 34.260 | 22.561 | 54.825 | 1.00 2 | 22.87 | | AAAA |
| | | C · | ALA | Δ | 148 | | 36.378 | 22.998 | 56.054 | 1.00 2 | 22.33 | | AAAA |
| ATO: | | | | | | | | | | | | | |
| ATO: | M 1160 | 0 | ALA | A | 148 | | 36.912 | 22.249 | 56.861 | 1.00 2 | 43.44 | | AAAA |
| | | N | VAL | Δ | 149 | | 37.050 | 23.661 | 55.122 | 1.00 | 22.50 | | AAAA - |
| ATO | | | | | | | | | | | | | |
| ATO | M 1162 | CA | VAL | А | 149 | | 38.505 | 23.569 | 55.018 | 1.00 | | | AAAA |
| ATO: | M 1163 | CB | VAL | A | 149 | | 39.066 | 24.581 | 54.002 | 1.00 2 | 20.46 | | AAAA |
| | | | | | | | | | | | | | AAAA |
| ATO: | M 1164 | CGI | VAL | А | 149 | | 40.578 | 24.607 | 54.085 | 1.00 | | | |
| ATO | M 1165 | CG2 | VAL | Α | 149 | | 38.608 | 24.229 | 52.593 | 1.00 | 20.03 | | AAAA |
| | | | | | | | | 23.848 | 56.367 | 1.00 2 | 21 49 | | AAAA |
| ATO: | M 1166 | С | VAL | | | | 39.164 | | | | | | |
| ATO: | M 1167 | 0 | VAL | А | 149 | | 40.147 | 23.197 | 56.735 | 1.00 | 22.11 | | AAAA |
| | | | - | | | | | | 57.088 | 1.00 2 | | | AAAA |
|) ATO | | N | GL. | | | | 38.628 | 24.826 | | | | | |
| ATO: | M 1169 | CA | GL. | Α | 150 | | 39.171 | 25.176 | 58.386 | 1.00 | 21.70 | • | AAAA |
| | | c · | GL. | | | | 38.973 | 24.043 | 59.368 | 1.00 | 22.31 | | AAAA |
| ATO | | | | | | | | | | | | | |
| ATO: | M 1171 | 0 | GLY | Α | 150 | | 39.913 | 23.597 | 60.026 | 1.00 2 | | | AAAA |
| | | N | ILE | Z) | 151 | | 37.736 | 23.566 | 59.453 | 1.00 2 | 22.86 | | AAAA |
| ATO | | | | | | | | | | | | | |
| ATO | M 1173 | CA | ILE | A | 151 | | 37.388 | 22.474 | 60.346 | 1.00 | | | AAAA |
| | | CB | ILE | | | | 35.894 | 22.124 | 60.191 | 1.00 | 21.51 | | AAAA |
| ATO: | | | | | | | | | | | | | |
| ATO | M 1175 | CG2 | ILE | A, | 151 | | 35.542 | 20.899 | 61.019 | 1.00 2 | | | AAAA |
| | | | ILE | | | | 35.051 | 23.329 | 60.627 | 1.00 2 | 20.39 | | AAAA |
| ATO: | | | | | | | | | | | | | |
| ATO | M 1177 | CD1 | ILE | Α | 151 | | 33.576 | 23.199 | 60.361 | 1.00 | | | AAAA |
| | | C | ILE | | | | 38.265 | 21.243 | 60.096 | 1.00 2 | 23.29 | | AAAA |
| ATO | | | | | | | | | | | | | |
| ATO: | M 1179 | 0 | ILE | Α | 151 | | 38.786 | 20.660 | 61.038 | 1.00 2 | 4588 | | AAAA |
| | | | GLU | 7 | 152 | | 38.435 | 20.853 | 58.836 | 1.00 2 | 24.13 | | AAAA |
| ATO | | N | CLU | n | 104 | | | | | | | | |
| ATO | y 1181 | CA | GLU | Α | 152 | | 39.267 | 19.697 | 58.5 17 | 1.00 2 | 25.01 | | AAAA |
| | | | GLU | 7. | 152 | | 39.242 | 19.404 | 57.010 | 1.00 2 | 25.07 | | AAAA |
| ATO | M 1182 | CB | | | | | | | | | | | |
| ATO | | CG | GLU | A | 152 | | 37.910 | 18.886 | 56.526 | 1.00 2 | 44.56 | | AAAA |
| | | | GLU | | | | 37.500 | 17.570 | 57.198 | 1.00 2 | 25.00 | | AAAA |
| ATO | M 1184 | CD | الارى | H | 136 | | | _ | | | | | |
| ATO | | OE1 | GLU | Α | 152 | | 36.345 | 17.158 | 57.011 | 1.00 2 | 40.40 | | AAAA |
| | | 023 | GLU | 2 | 152 | | 38.315 | 16.935 | 57.897 | 1.00 2 | 25.00 | | AAAA |
| ATO | y 1186 | OE2 | كابلاف | 4 | 102 | | | | | | | | |
| ATO | | С | GLU | Α | 152 | | 40.694 | 19.957 | 58.965 | 1.00 | 40.06 | | AAAA |
| | | | GLU | 7 | 152 | | | | 59.331 | 1.00 | 26.40 | | AAAA |
| ATO | M 1188 | 0 | GTO | ~ | 104 | | 41.425 | 19.035 | | | | • | * M = M . |
| | | | | | | | | | | | | | - |

Figure 19-19

| | | | | _ | | | | |
|--------|------|-----|------------------|----------|--------|--------|------------|-------------|
| MOTA | 1189 | N | TYR A 15 | 3 41.085 | 21.225 | 58.925 | 1.00 27.30 | AAAA |
| MOTA | 1190 | CA | TYR A 15 | 3 42.422 | 21.632 | 59.334 | 1.00 27.63 | AAAA |
| ATOM | 1191 | CB | TYR A 15 | | 23.153 | 59.268 | 1.00 26.99 | AAAA |
| | 1192 | CG | TYR A 15 | _ | | 59.710 | 1.00 27.03 | |
| MOTA | | | | | | | | AAAA |
| MOTA | 1193 | CD: | | 3 44.942 | 23.790 | 58.837 | 1.00 27.78 | AAAA |
| ATOM | 1194 | CE: | l TYR A 15 | 3 46.165 | 24.356 | 59.250 | 1.00 28.40 | AAAA |
| ATOM | 1195 | CD2 | | | 24.215 | 61.007 | 1.00 27.52 | AAAA |
| | | | | | | | | |
| MOTA | 1196 | CE | | | 24.774 | 61.425 | 1.00 27.66 | AAAA |
| MOTA | 1197 | CZ | TYR A 15 | 3 46.284 | 24.845 | 60.547 | 1.00 28.15 | AAAA |
| ATOM | 1198 | OH | TYR A 15 | 3 47.457 | 25.407 | 60.974 | 1.00 28.83 | AAAA |
| MOTA | 1199 | С | TYR A 15 | | 21.172 | 60.769 | 1.00 27.82 | • |
| | | | | | | | | AAAA |
| MOTA | 1200 | 0 | TYR A 15 | | 20.552 | 61.110 | 1.00 27.15 | AAAA |
| -MOTA | 1201 | N | LEU A 15 | 41.636 | 21.487 | 61.604 | 1.00 29.25 | AAAA . |
| MOTA | 1202 | CA | LEU A 15 | 41.665 | 21.138 | 63.014 | 1.00 29.35 | AAAA |
| | 1203 | CB | LEU A 15 | | 21.829 | 63.715 | 1.00 30.25 | AAAA |
| MOTA | | | | | | | | |
| MOTA | 1204 | CG | LEU A 15 | | 23.346 | 63.792 | 1.00 31.10 | AAAA |
| ATOM | 1205 | CDI | LEU A 15 | 1 39.348 | 24.020 | 64.092 | 1.00 31.24 | AAAA |
| MOTA | 1206 | CD2 | LEU A 15 | 41.747 | 23.669 | 64.852 | 1.00 29.84 | AAAA |
| ATOM | 1207 | C | LEU A 15 | | 19.639 | 63.263 | 1.00 29.73 | AAAA |
| | | | | | | | | |
| ATOM | 1208 | 0 | LEU A 15 | | 19.151 | 64.150 | 1.00 30.51 | AAAA |
| MOTA | 1209 | И | ARG A 15 | 40.832 | 18.903 | 62.489 | 1.00 28.95 | AAAA |
| MOTA | 1210 | CA | ARG A 15 | 40.771 | 17.459 | 62.671 | 1.00 28.94 | AAAA |
| ATOM | 1211 | CB | ARG A 15 | | 16.820 | 61.723 | 1.00 28.64 | AAAA |
| | | | | | | | | |
| ATOM | 1212 | CG | ARG A 15 | | 17.312 | 61.952 | 1.00 27.82 | AAAA |
| MOTA | 1213 | CD | ARG A 15 | 37.319 | 16.751 | 60.955 | 1.00 27.19 | AAAA |
| ATOM | 1214 | ΝE | ARG A 159 | 36.804 | 15.444 | 61.338 | 1.00 28.86 | AAAA |
| MOTA | 1215 | CZ | ARG A 159 | 35.939 | 14.742 | 60.612 | 1.00 28.93 | AAAA |
| ATOM | 1216 | | ARG A 15 | | 15.227 | 59.459 | 1.00 29.47 | AAAA |
| | | | | | | | | |
| ATOM | 1217 | | ARG A 155 | | 13.574 | 61.053 | 1.00 28.76 | AAAA |
| ATOM | 1218 | С | ARG A 155 | 42.158 | 16.853 | 62.438 | 1.00 30.20 | AAAA |
| ATOM | 1219 | 0 | ARG A 155 | 42.572 | 15.949 | 63.164 | 1.00 30.74 | AAAA |
| ATOM | 1220 | N | LYS A 156 | | 17.362 | 61.447 | 1.00 30.32 | AAAA |
| | 1221 | CA | LYS A 156 | | 16.838 | 61.173 | 1.00 30.07 | |
| MOTA | | | | | | | | AAAA |
| MOTA | 1222 | CB | LYS A 156 | | 17.373 | 59.847 | 1.00 30.26 | AAAA |
| ATOM . | 1223 | CG | LYS A 156 | 46.168 | 16.869 | 59.525 | 1.00 30.16 | AAAA |
| ATOM | 1224 | CD | LYS A 156 | 46.686 | 17.368 | 58.181 | 1.00 31.19 | AAAA |
| ATOM | 1225 | CE | LYS A 156 | | 16.813 | 56.986 | 1.00 31.70 | AAAA |
| | | | | | | | | |
| ATOM | 1226 | NZ | LYS A 156 | | 15.324 | | 1.00 31.20 | AAAA |
| MOTA | 1227 | С | LYS A 156 | | 17.202 | 62.306 | 1.00 30.08 | AAAA |
| MOTA | 1228 | 0 | LYS A 156 | 46.192 | 16.550 | 62.485 | 1.00 29.16 | · AAAA |
| ATOM | 1229 | N | LYS A 157 | 44.816 | 18.252 | 63.053 | 1.00 30.08 | AAAA |
| | 1230 | CA | LYS A 157 | | 18.691 | 64.196 | 1.00 31.03 | AAAA |
| MOTA | | | | | | | | |
| MOTA | 1231 | CB | LYS A 157 | | | 64.452 | 1.00 31.81 | AAAA |
| ATOM | 1232 | CG | LYS A 157 | 46.067 | 21.134 | 63.419 | 1.00 32.12 | AAAA |
| ATOM | 1233 | CD | LYS A 157 | 47.580 | 21.041 | 63.348 | 1.00 31.34 | AAAA |
| ATOM | 1234 | CE. | LYS A 157 | 48.080 | 21.941 | 62.226 | 1.00 32.66 | NAAA |
| | | | | 49.556 | 21.921 | 61.996 | 1.00 32.74 | |
| MOTA | 1235 | NZ | LYS A 157 | | | | | ,AAA |
| MOTA | 1236 | С | LYS A 157 | 45.196 | 17.923 | 65.458 | 1.00 31.73 | . YAAA |
| ATOM | 1237 | O· | LYS A 157 | 45.652 | 18.230 | 66.558 | 1.00 31.93 | AAAA |
| ATOM | 1238 | N | GLY A 158 | 44.312 | 16.942 | 65.299 | 1.00 32.41 | AAAA |
| | 1239 | CA | GLY A 158 | 43.901 | 16.140 | 66.436 | 1.00 32.34 | AAAA |
| ATOM | | | | | | | | |
| MOTA | 1240 | С | GLY A 158 | 42.604 | 16.429 | 67.172 | 1.00 32.65 | AAAA |
| MOTA | 1241 | 0 | GLY A 158 | 42.182 | 15.604 | 67.980 | 1.00 32.85 | AAAA |
| ATOM | 1242 | N | PHE A 159 | 41.960 | 17.565 | 66.932 | 1.00 33.16 | AAAA |
| | | | | 40.712 | | 67.650 | 1.00 34.16 | AAAA |
| ATOM | 1243 | CA | PHE A 159 | | 17.842 | | | |
| MOTA | 1244 | CB | PHE A 159 | 40.220 | 19.281 | 67.403 | 1.00 34.81 | AAAA |
| ATOM | 1245 | CG | PHE A 159 | 41.134 | 20.343 | 67.965 | 1.00 34.01 | AAAA |
| ATOM | 1246 | | PHE A 159 | 42.327 | 20.669 | 67.329 | 1.00 34.18 | AAAA |
| | | CD3 | PHE A 159 | 40.821 | 20.981 | 69.166 | 1.00 34.61 | AAAA |
| MOTA | 1247 | | | | | | | |
| MOTA | 1248 | | PHE A 159 | 43.197 | 21.610 | 67.874 | 1.00 33.65 | AAAA |
| ATOM: | 1249 | CE2 | PHE A 159 | 41.689 | 21.924 | 69.718 | 1.00 34.52 | AAAA |
| MOTA | 1250 | CZ | PHE A 159 | 42.878 | 22.236 | 69.065 | 1.00 33.90 | AAAA |
| | 1251 | | PHE A 159 | 39.645 | 16.840 | 67.239 | 1.00 34.04 | AAAA |
| ATOM | | C | | | | | | |
| ATOM | 1252 | | PHE A 159 | 39.568 | 16.456 | 66.068 | 1.00 34.98 | AAAA |
| MOTA | 1253 | | LYS A 160 | 38.839 | 16.403 | 68.202 | 1.00 33.36 | AAAA |
| ATOM | 1254 | | LYS A 160 | 37.794 | 15.415 | 67.936 | 1.00 33.11 | AAAA |
| | | | | • | | • | | _ |

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| MOTA | 1255 | CB | LYS | Α | 160 | | 38.060 | 14.140 | 68.763 | 1.00 33.97 | AAAA |
|------|------|-----|-----|---|------------|---|--------|--------|------------------|------------|--------------|
| MOTA | 1256 | CG | • | | 160 | | 39.410 | 13.491 | 68.457 | 1.00 35.31 | AAAA |
| ATOM | 1257 | CD | | | 160 | | 39.833 | 12.364 | 69.429 | 1.00 36.48 | AAAA |
| ATOM | 1258 | CE | | | 160 | | 39.095 | 11.037 | 69.243 | 1.00 37.97 | AAAA |
| MOTA | 1259 | NZ | | | 160 | | 37.636 | 11.080 | 69.568 | 1.00 39.67 | AAAA |
| MOTA | 1260 | C | | | 160 | | 36.385 | 15.941 | 68.210 | 1.00 31.68 | AAAA |
| | 1261 | ō | | | 160 | | 35.405 | 15.290 | 67.887 | 1.00 31.51 | AAAA |
| ATOM | 1262 | N | | | 161 | | 36.291 | 17.114 | 68.819 | 1.00 31.11 | AAAA |
| ATOM | 1263 | CA | | | 161 | * | 35.003 | 17.719 | 69.114 | 1.00 30.92 | AAAA |
| MOTA | 1264 | CB | | | 161 | | 34.655 | 17.592 | 70.604 | 1.00 31.78 | AAAA |
| MOTA | | CG | | | 161 | | 34.451 | 16.157 | 71.102 | 1.00 32.91 | AAAA |
| MOTA | 1265 | CD | | | 161 | | 33.994 | 16.126 | 72.570 | 1.00 33.26 | AAAA |
| ATOM | 1266 | NE | | | 161 | | 34.929 | 16.797 | 73.476 | 1.00 34.01 | AAAA |
| MOTA | 1267 | CZ | | | 161 | | 36.183 | 16.404 | 73.698 | 1.00 34.88 | AAAA |
| ATOM | 1268 | | ARG | | | | 36.675 | 15.334 | 73.081 | 1.00 34.89 | AAAA |
| ATOM | 1269 | | ARG | | | | 36.954 | 17.084 | 74.537 | 1.00 34.71 | AAAA |
| ATOM | 1270 | | | | | | 35.061 | 19.185 | 68.714 | 1.00 30.28 | AAAA |
| ATOM | 1271 | C | | | 161 161 | | 35.365 | 20.059 | 69.529 | 1.00 29.86 | AAAA |
| ATOM | 1272 | 0 | | | | | 34.774 | 19.433 | 67.437 | 1.00 28.86 | |
| ATOM | 1273 | N | | | 162 | | 34.788 | 20.774 | 66.862 | 1.00 26.41 | AAAA |
| MOTA | 1274 | CA | | | 162 | | | 20.762 | 65.464 | 1.00 26.87 | AAAA |
| ATOM | 1275 | CB | | | 162 | | 35.443 | | 64.872 | 1.00 26.91 | AAAA |
| MOTA | 1276 | | ILE | | | | 35.453 | 22.160 | 65.578 | 1.00 28.19 | AAAA |
| ATOM | 1277 | | ILE | | | | 36.877 | 20.234 | 64.240 | 1.00 28.19 | AAAA |
| MOTA | 1278 | | ILE | | | | 37.614 | 20.090 | | | AAAA |
| MOTA | 1279 | С | | | 162 | | 33.369 | 21.283 | 66.731 | 1.00 24.08 | |
| MOTA | 1280 | 0 | | | 162 | | 32.485 | 20.572 | 66.267 | 1.00 24.40 | AAAA |
| ATOM | 1281 | N | | | 163 | | 33.153 | 22.519 | 67.153 | 1.00 22.25 | AAAA |
| MOTA | 1282 | CA | | | 163 | • | 31.838 | 23.126 | 67.074 | 1.00 20.48 | AAAA |
| ATOM | 1283 | CB | | | 163 | | 31.408 | 23.671 | 68.440 | 1.00 20.97 | AAAA |
| MOTA | 1284 | CG | | | 163 | | 30.099 | 24.477 | 68.486 | 1.00 20.50 | AAAA |
| MOTA | 1285 | | LEU | | | | 28.998 | 23.695 | 67.799 | 1.00 19.07 | AAAA |
| ATOM | 1286 | CD2 | LEU | | | | 29.738 | 24.802 | 69.950 | 1.00 19.76 | AAAA |
| MOTA | 1287 | С | | | 163 | | 31.801 | 24.241 | 66.055 | 1.00 18.76 | AAAA |
| MOTA | 1288 | 0 | | | 163 | | 32.756 | 24.986 | 65.894 | 1.00 18.41 | AAAA |
| MOTA | 1289 | N | TYR | A | 164 | | 30.677 | 24.344 | 65.368 | 1.00 17.85 | AAAA |
| ATOM | 1290 | CA | | | 164 | | 30.496 | 25.372 | 64.373 | 1.00 17.16 | AAAA |
| ATOM | 1291 | CB | | | 164 | | 30.644 | 24.768 | 62.983 | 1.00 17.45 | AAAA |
| ATOM | 1292 | CG | | | 164 | | 30.484 | 25.783 | 61.900 | 1.00 17.70 | AAAA |
| ATOM | 1293 | | TYR | | | | 31.444 | | 61.701 | 1.00 16.23 | AAAA |
| ATOM | 1294 | | TYR | | | | 31.280 | 27.734 | 60.721 | 1.00 17.35 | AAAA |
| MOTA | 1295 | | TYR | | | | 29.350 | 25.781 | 61.092 | 1.00 17.95 | AAAA |
| ATOM | 1296 | CE2 | TYR | | | | 29.173 | 26.746 | 60.103 | 1.00 18.03 | AAAA AAAA |
| ATOM | 1297 | CZ | | | 164 | | 30.138 | 27.717 | 59.919 | 1.00 17.30 | |
| MOTA | 1298 | OH | | | 164 | | 29.955 | 28.647 | 58.926 | 1.00 16.70 | AAAA |
| MOTA | 1299 | С | | | 164 | | 29.123 | 26.016 | 64.514 | 1.00 15.85 | AAAA AAAA |
| MOTA | 1300 | 0 | | | 164 | • | 28.101 | 25.351 | 64.416 64.743 | 1.00 16.44 | AAAA |
| ATOM | 1301 | N | | | 165 | | 29.115 | 27.319 | | 1.00 15.54 | |
| MOTA | 1302 | CA | | | 165 • | • | 27.878 | 28.088 | 64.897 | 1.00 15.71 | AAAA AAAA |
| ATOM | 1303 | CB | | | 165 | | 27.869 | 28.819 | 66.250 | 1.00 15.18 | |
| ATOM | 1304 | CG2 | ILE | A | 165 | | 26.621 | 29.685 | 66.374 | 1.00 13.94 | AAAA |
| ATOM | 1305 | CG1 | ILE | A | 165 | | 20.000 | | 67.386 | | AAAA |
| ATOM | 1306 | CD1 | ILE | A | 165 | | 28.356 | 28.421 | 68.747 | 1.00 13.94 | AAAA |
| ATOM | 1307 | С | ILE | A | 165 | | 27.808 | 29.124 | 63.754 | 1.00 16.00 | AAAA |
| ATOM | 1308 | 0 | ILE | Α | 165 | | 28.711 | 29.941 | 63.576 | 1.00 16.56 | AAAA |
| ATOM | 1309 | N | ASP | Α | 166 | ~ | 26.721 | 29.087 | 63.001 | 1.00 16.18 | AAAA |
| ATOM | 1310 | CA | ASP | Ά | 166 | | 26.524 | 29.962 | 61.865 | 1.00 16.67 | AAAA |
| MOTA | 1311 | CB | | | 166 | | 26.240 | 29.066 | 60.651 | 1.00 18.05 | AAAA |
| MOTA | 1312 | CG | ASP | A | 166 | | 26.238 | 29.809 | 59.329 | 1.00 19.21 | AAAA |
| ATOM | 1313 | | ASP | | | | 25.353 | 30.659 | 59.114 | 1.00 18.36 | AAAA |
| ATOM | 1314 | | ASP | | | | 27.131 | 29.521 | 58.495 | 1.00 19.19 | AAAA |
| ATOM | 1315 | c | | | 166 | | 25.342 | 30.904 | 62.169 | 1.00 17.57 | AAAA |
| | 1316 | ō | | | 166 | | 24.206 | 30.459 | 62.321 | 1.00 17:26 | AAAA |
| ATOM | 1317 | N . | | | 167 | | 25.605 | 32.202 | 62.274 | 1.00 16.67 | AAAA |
| ATOM | 1318 | CA | | | 167 | | 24.526 | 33.135 | 62.562 | 1.00 16.89 | AAAA |
| MOTA | 1318 | CB | | | 167 | | 24.923 | 34.116 | 63.663 | 1.00 17.27 | AAAA |
| MOTA | | CG | | | 167 | | 25.499 | 33.529 | 64.954 | 1.00 18.37 | AAAA |
| ATOM | 1320 | | | | **** | | | | • | | |
| • | | | | 4 | * | | | | | | |

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| ATOM | 1321 | CD1 LEU A 167 | 25.760 | 34.671 | 65.933 | 1.00 18.72 | AAAA |
|--------------|--------------------|------------------------|------------------|------------------|------------------|--------------------------|-------------------|
| MOTA | 1322 0 | CD2 LEU A 167 | 24.566 | 32.507 | 65.547 | 1.00 17.06 | AAAA |
| MOTA | 1323 (| LEU A 167 | 24.146 | 33.897 | 61.307 | 1.00 17.18 | AAAA |
| MOTA | 1324 0 | | 23.390 | 34.850 | 61.358 | 1.00 17.21 | AAAA |
| MOTA | 1325 N | | 24.683 | 33.457 | 60.178 | 1.00 17.83 | AAAA |
| ATOM | 1326 C | A ASP A 168 | 24.382 | 34.067 | 58.904 | 1.00 17.84 | AAAA |
| ATOM | | B ASP A 168 | 25.178 | 33.397 | 57.807 | 1.00 20.42 | AA A A |
| MOTA | | G ASP A 168 | 25.140 | | 56.529 | 1.00 21.41 | AAAA |
| ATOM | 1329 C | : ASP A. 168 | 22.915 | 33.783 | 58.660 | 1.00 18.35 | AAAA |
| MOTA | 1330 C | | 22.419 | 32.722 | 59.032 | 1.00 19.62 | AAAA |
| MOTA | | D1 ASP A 168 | - 26.066 | 34.972 | 56.330 | 1.00 22.42 | AAAA |
| ATOM | | D2 ASP A 168 | 24.186 | 33.971 | 55.746 | 1.00 21.79 | AAAA |
| MOTA | 1333 N | | 22.239 | 34.717 | | 1.00 17.98 | AAAA |
| MOTA | | A ALA A 169 | 20.824 | 34.601 | 57.708 | 1.00 17.36 | AAAA |
| MOTA | | B ALA A 169 | 20.348 | 35.860 | 57.007 | 1.00 17.00 | AAAA |
| MOTA | 1336 C | | 20.439 | 33.377 | 56.887 | 1.00 18.64 | AAAA |
| ATOM | 1337 0 | | 19.255 | 33.043 | 56.819 | 1.00 19.46 | AAAA |
| MOTA | 1338 N | | 21.412 | 32.712 | 56.262 | 1.00 18.71 | AAAA |
| MOTA | 1339 C | | 21.107 | 31.518 | 55.464 | 1.00 18.43 | AAAA |
| MOTA | 1340 C | | 21.802 | 30.265 | 55.986 | 1.00 18.02 | AAAA |
| MOTA | 1341 O 1342 C | | 22.910 | 30.332 | 56.514 | 1.00 17.20 | AAAA |
| ATOM ATOM | 1342 C | | 21.539 21.137 | 31.678 | 54.004 | 1.00 18.79 | AAAA |
| ATOM | | D1 HIS A 170 | 21.137 | 32.968 34.162 | 53.386 | 1.00 17.65 | AAAA |
| ATOM | | E1 HIS A 170 | 21.112 | 35.081 | 53.828 53.054 | 1.00 18.08 | AAAA |
| ATOM | | D2 HIS A 170 | 20.301 | 33.194 | 52.348 | 1.00 18.95 1.00 18.81 | AAAA |
| ATOM | | E2 HIS A 170 | 20.291 | 34.544 | 52.140 | 1.00 19.66 | AAAA AAAA |
| ATOM | 1348 N | | 21.142 | 29.124 | 55.793 | 1.00 17.53 | AAAA |
| ATOM | 1349 C | | 21.662 | 27.822 | 56.193 | 1.00 16.38 | AAAA |
| ATOM | 1350 CI | B HIS A 171 | 20.644 | 26.740 | 55.830 | 1.00 16.32 | AAAA |
| MOTA | 1351 C | G HIS A 171 | 21.157 | 25.337 | 55.958 | 1.00 15.91 | AAAA |
| MOTA | 1352 CI | 02 HIS A 171 | 21.241 | 24.336 | 55.051 | 1.00 14.14 | AAAA |
| ATOM | 1353 NI | D1 HIS A 171 | 21.602 | 24.807 | 57.151 | 1.00 16.79 | AAAA |
| ATOM | | E1 HIS A 171 | 21.937 | 23.543 | 56.973 | 1.00 14.91 | AAAA |
| ATOM | | E2 HIS A 171 | 21.725 | 23.234 | 55.709 | 1.00 15.45 | AAAA |
| MOTA | 1356 C | HIS A 171 | 22.982 | 27.522 | 55.509 | 1.00 16.94 | AAAA |
| MOTA | 1357 0 | HIS A 171 | 23.146 | 27.725 | 54.318 | 1.00 18.71 | AAAA |
| ATOM | 1358 N 1359 CA | CYS A 172 | 23.926 | 27.019 | 56.279 | 1.00 16.99 | AAAA |
| MOTA MOTA | 1359 CA 1360 CE | | 25.237 26.219 | 26.670 26.721 | 55.778 56.947 | 1.00 16.23 | AAAA |
| ATOM | 1361 SG | | 25.638 | 25.773 | 58.397 | 1.00 17.89 1.00 17.89 | AAAA AAAA |
| ATOM | 1362 C | CYS A 172 | 25.205 | 25.271 | 55.210 | 1.00 17.03 | AAAA |
| ATOM | 1363 0 | CYS A 172 | 25.947 | 24.413 | 55.670 | 1.00 17.66 | AAAA |
| ATOM | 1364 N | ASP A 173 | 24.364 | 25.026 | 54.214 | 1.00 18.25 | AAAA |
| ATOM | 1365 CA | | 24.253 | 23.680 | 53.620 | 1.00 19.91 | AAAA |
| ATOM | 1366 CB | ASP A 173 | 23.342 | 23.699 | 52.397 | 1.00 20.86 | AAAA |
| MOTA | 1367 CG | ASP A 173 | 23.780 | 24.719 | 51.358 | 1.00 21.90 | AAAA |
| MOTA | 1368 OD | 1 ASP A 173 | 23.257 | 24.640 | 50.217 | 1.00 21.35 | AAAA |
| MOTA | .1369 OD | 2 ASP A 173 | 24.624 | 25.597 | 51.687 | 1.00 21.35 | AAAA |
| MOTA | 1370 C´ | ASP A 173 | 25.573 | 23.021 | 53.227 | 1.00 21.02 | AAAA |
| ATOM | 1371 0 | ASP A 173 | 25.673 | 21.785 | 53.199 | 1.00 22.79 | AAAA |
| MOTA | 1372 N | GLY A 174 | 26.579 | 23.832 | 52.912 | 1.00 20.03 | AAAA |
| ATOM | 1373 CA | | 27.870 | 23.277 | 52.553 | 1.00 19.72 | AAAA |
| ATOM | 1374 C | GLY A 174 | 28.537 | 22.680 | 53.771 | 1.00 20.27 | AAAA |
| ATOM | 1375 0 | GLY A 174 | 29.110 | 21.599 | 53.711 | 1.00 19.77 | AAAA |
| ATOM | 1376 N | VAL A 175 | 28.448 | 23.387 | 54.893 | 1.00 21.38 | AAAA |
| ATOM | 1377 CA | VAL A 175 | 29.056 | 22.934 | 56.135 | 1.00 22.26 | AAAA |
| ATOM | 1378 CB | VAL A 175 | 29.032 | 24.040 | 57.203 | 1.00 23.15 | AAAA |
| ATOM | | 1 VAL A 175 | 29.853 | 23.617 | 58.418 | 1.00 22.84 | AAAA |
| ATOM | | 2 VAL A 175 | 29.562 | | .56.612 | 1.00 23.43 | AAAA |
| ATOM · | 1381 C | VAL A 175 VAL A 175 | 28.302 28.893 | 21.724 | 56.654 57.210 | 1.00 23.51 1.00 23.74 | AAAA |
| ATOM | 1382 O 1383 N | GLN A 176 | 26.993 | 20.803 21.721 | 56.452 | 1.00 23.74 | AAAA |
| ATOM ATOM | 1383 N 1384 CA | GLN A 176 | 26.171 | 20.601 | 56.893 | 1.00 25.41 | AAAA AAAA |
| ATOM | 1385 CB | GLN A 176 | 24.689 | 20.913 | 56.694 | 1.00 24.77 | AAAA |
| MOTA | 1386 CG | GLN A 176 | 23.799 | 19.735 | 57.036 | 1.00 26.23 | AAAA |
| | | | | | 2 | | |

| | | | | | | | | • | |
|--------------|--------------|----------|--------|-----|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 1387 | CD | GLN A | 176 | 22.334 | 20.094 | 57.069 | 1.00 27.17 | AAAA |
| ATOM | 1388 | OE1 | GLN A | | 21.902 | 20.879 | 57.911 | 1.00 28.24 | AAAA |
| MOTA | 1389 | NE2 | GLN A | 176 | 21.556 | 19.522 | 56.151 | 1.00 26.54 | AAAA |
| ATOM | 1390 | C | GLN A | | 26.512 | 19.293 | 56.180 | 1.00 25.67 | AAAA |
| ATOM | 1391 | 0 | GLN A | | 26.789 | 18.285 | 56.820 | 1.00 26.98 | AAAA |
| MOTA | 1392 | N | GLU A | | 26.490 | 19.309 | 54.853 | 1.00 26.34 | AAAA |
| MOTA | 1393 | CA | GLU A | | 26,786 | 18.117 | 54.073 | 1.00 26.18 | AAAA |
| MOTA | 1394 | CB | GLU A | | 26.746 | 18.468 | 52.580 | 1.00 27.13 | AAAA |
| ATOM | 1395 | CG | GLU A | | 26.769 | 17.269 | 51.628 | 1,00 29.77 | AAAA |
| ATOM | 1396 | CD | .GLU A | | 26.623 | 17.660 | 50.147 | 1.00 31.29 | AAAA |
| ATOM | 1397 | | GLU A | | 27.655 | 17.935 | 49.500 | 1.00 31.35 | AAAA |
| ATOM | 1398 | | GLU A | | 25.471 | 17.703 | 49.636 | 1.00 32.05 | AAAA |
| MOTA | 1399 | C | GLU A | | 28.160 | 17.556 | 54.460 | 1.00 26.38 | AAAA |
| MOTA | 1400 | õ | GLU A | | 28.338 | 16.349 | 54.595 | 1.00 25.41 | AAAA |
| ATOM | 1401 | N | ALA A | | 29.115 | 18.458 | 54.659 | 1.00 -27.58 | AAAA |
| ATOM | 1402 | CA | ALA A | | 30.495 | 18.119 | 55.004 | 1.00 27.66 | - AAAA |
| MOTA | 1403 | CB | ALA A | | 31.345 | 19.385 | 54.994 | 1.00 26.20 | AAAA |
| ATOM | 1404 | C | ALA A | | 30.713 | 17.370 | 56.318 | 1.00 28.33 | AAAA |
| ATOM | 1405 | ō | ALA A | | 31.685 | 16.626 | 56.439 | 1.00 29.44 | AAAA |
| ATOM | 1406 | N | PHE A | | 29.849 | 17.564 | 57.308 | 1.00 28.25 | AAAA |
| MOTA | 1407 | CA | PHE A | | 30.036 | 16.852 | 58.561 | 1.00 29.20 | AAAA |
| MOTA | 1408 | CB | PHE A | 179 | 30.570 | 17.794 | 59.624 | 1.00 29.35 | AAAA |
| MOTA | 1409 | CG | PHE A | 179 | 31.751 | 18.572 | 59.171 | 1.00 30.26 | AAAA |
| ATOM | 1410 | CD1 | PHE A | 179 | 31.582 | 19.777 | 58.497 | 1.00 31.01 | AAAA |
| MOTA | 1411 | CD2 | PHE A | 179 | 33.033 | 18.069 | 59.339 | 1.00 30.37 | AAAA |
| ATOM | 1412 | CE1 | PHE A | 179 | 32.670 | 20.470 | 57.993 | 1.00 31.20 | AAAA |
| MOTA | 1413 | CE2 | PHE A | 179 | 34.133 | 18.749 | 58.840 | 1.00 31.74 | AAAA |
| ATOM | 1414 | CZ | PHE A | 179 | 33.950 | 19.960 | 58.161 | 1.00 31.81 | AAAA |
| ATOM | 1415 | С | PHE A | 179 | 28.760 | 16.180 | 59.040 | 1.00 30.33 | AAAA |
| ATOM | 1416 | 0 | PHE A | 179 | 28.624 | 15.810 | 60.215 | 1.00 31.82 | AAAA |
| MOTA | 1417 | N | TYR A | 180 | 27.842 | 15.994 | 58.105 | 1.00 29.18 | AAAA |
| ATOM | 1418 | CA | TYR A | 180 | 26.564 | 15.379 | 58.389 | 1.00 28.99 | AAAA |
| MOTA | 1419 | CB | TYR A | | 25.725 | 15.343 | 57.123 | 1.00 28.30 | AAAA |
| ATOM | 1420 | CG | TYR A | | | 15.422 | 57.384 | 1.00 28.27 | AAAA |
| MOTA | 1421 | | TYR A | | 23.392 | 14.386 | 57.021 | 1.00 27.05 | AAAA |
| ATOM | 1422 | | TYR A | | 22.029 | 14.491 | 57.197 | 1.00 28.51 | AAAA |
| ATOM | 1423 | CD2 | TYR A | | 23.686 | 16.573 | 57.942 | 1.00 29.34 | AAA |
| MOTA | 1424 | CE2 | TYR A | | 22.316 | 16.691 | 58.125 | 1.00 29.27 | AAAA |
| MOTA | 1425 | CZ | TYR A | | 21.495 | 15.645 | 57.746 57.893 | 1.00 29.33 1.00 30.83 | AAAA AAAA |
| MOTA | 1426 | ОН | TYR A | | 20.141 | 15.775 13.970 | 58.940 | 1.00 30.83 | AAAA |
| MOTA | 1427 | C | TYR A | | 26.673 | 13.577 | 59.785 | 1.00 28.71 | AAAA |
| MOTA | 1428 | 0 | TYR A | | 25.877 27.662 | 13.214 | 58.472 | 1.00 29.03 | AAAA |
| MOTA | 1429 | N | ASP A | | 27.802 | 11.828 | 58.914 | 1.00 28.49 | AAAA |
| MOTA | 1430 | CA CB | ASP A | | 28.140 | 10.930 | 57.715 | 1.00 27.59 | AAAA |
| ATOM | 1431 1432 | CG | ASP A | | 29.548 | 11 122 | 57.229 | 1.00 28.82 | AAAA |
| MOTA | 1432 | | ASP A | | 29:981 | 12 292 | 57.183 | 1.00 29.25 | AAAA |
| ATOM | 1434 | | ASP A | | | ,10 119 | 56.887 | 1.00 28.68 | AAAA |
| ATOM | 1435 | C | ASP A | | 28.863 | 11.631 | 60.009 | 1.00 27.67 | AAAA |
| ATOM | 1436 | ō | ASP A | | 29.271 | 10.504 | 60.293 | 1.00 27.57 | AAAA |
| atom Atom | 1437 | N | THR A | | | 12.713 | 60.628 | 1.00 26,27 | AAAA |
| MOTA | 1438 | CA | THR A | | 30.284 | 12.544 | 61.689 | 1.00 26.22 | AAAA |
| ATOM | 1439 | CB | THR A | | 31.670 | 13.118 | 61.317 | 1.00 25.92 | AAAA |
| ATOM | 1440 | | THR A | | 32.564 | 12.935 | 62.416 | 1.00 25,06 | AAAA |
| ATOM | 1441 | | THR A | | 31.577 | 14.594 | 60.974 | 1.00 25.25 | AAAA |
| ATOM | 1442 | c | THR A | | 29.792 | 13.223 | 62.934 | 1.00 25.87 | AAAA |
| ATOM | 1443 | ō | THR A | | 28.942 | 14.102 | 62.863 | 1.00 26.35 | AAAA |
| ATOM | 1444 | N | ASP A | | 30.327 | 12.804 | 64.071 | 1.00 25.86 | AAAA |
| ATOM | 1445 | CA | ASP A | | 29.953 | 13.370 | 65.355 | 1.00 26.12 | AAAA |
| ATOM | 1446 | CB | ASP A | 183 | 29.468 | 12.260 | 66.274 | 1.00 27.10 | AAAA |
| ATOM | 1447 | CG | ASP A | | 30.515 | 11.194 | 66.488 | 1.00 28.80 | AAAA |
| ATOM | 1448 | OD1 | ASP A | | 31.063 | 10.691 | 65.480 | 1.00 29.78 | AAAA |
| ATOM | 1449 | OD2 | ASP A | 183 | 30.781 | 10.852 | 67.657 | 1.00 29.21 | AAAA |
| ATOM | 1450 | c | ASP A | 183 | 31.126 | 14.120 | 65.995 | 1.00 26.77 | AAAA |
| ATOM | 1451 | ō | ASP A | | 31.034 | 14.566 | 67.146 | 1.00 26.65 | AAAA |
| TOM | 1452 | N | GLN A | | 32.229 | | 65.254 | 1.00 26.05 | AAAA |

1452 N GLN A 184 32.229 14.254 65.254 1.00 26.05 SUBSTITUTE SHEET (RULE 26)

| 3 00011 | 1453 | | ~~ ~~ ~ | 104 | | | | | | |
|---------|------|------|---------|-----|----------------|--------|--------|--------|-------|--------|
| MOTA | 1453 | | GLN A | 184 | 33.381 | 14.983 | 65.766 | 1.00 | 25.85 | AAAA |
| ATOM | 1454 | CB | GLN A | 184 | 34.674 | 14.510 | 65.095 | 1.00 | 26 30 | AAAA |
| ATOM | 1455 | CG | GLN A | 184 | 34.920 | | 65.303 | 1.00 | | |
| ATOM | 1456 | CD | GLN A | | 36.273 | | | | | AAAA |
| | | | | | | | 64.822 | 1.00 | 28.40 | AAAA |
| ATOM | 1457 | | GLN A | | 36.685 | | 63.709 | 1.00 | 30.05 | AAAA |
| MOTA | 1458 | NE2 | GLN A | 184 | 36.970 | 11.816 | 65.651 | 1.00 | | AAAA |
| MOTA | 1459 | С | GLN A | | 33.159 | | 65.536 | | | |
| ATOM | 1460 | ŏ | | | | | | 1.00 | | AAAA |
| | | | GLN A | | 33.734 | | 66.220 | 1.00 | 24.57 | AAAA |
| MOTA | 1461 | N | VAL A | 185 | 32.290 | 16.791 | 64.584 | 1.00 | 25.17 | AAAA |
| ATOM | 1462 | CA | VAL A | 185 | 31.975 | 18.182 | 64.291 | 1.00 | | |
| ATOM | 1463 | CB | VAL A | | 32.324 | 18.563 | | | | AAAA |
| | | | | | | | 62.832 | 1.00 | | AAAA |
| MOTA | 1464 | | VAL A | | 32.045 | | 62.599 | 1.00 | 19.72 | AAAA |
| ATOM | 1465 | CG2 | VAL A | 185 | 33. <i>777</i> | 18.205 | 62.543 | 1.00 | 20.67 | AAAA . |
| MOTA | 1466 | C . | VAL A | 185 | 30.494 | 18.421 | 64.501 | 1.00 | | |
| ATOM | 1467 | 0 | VAL A | | 29.664 | 17.787 | 63.844 | | | AAAA |
| | | | | | | | | 1.00 | | AAAA |
| MOTA | 1468 | N | PHE A | | 30.162 | 19.311 | 65.434 | 1.00 | 23.40 | AAAA |
| ATOM | 1469 | CA | PHE A | 186 | 28.768 | 19.645 | 65.684 | 1.00 | 20.31 | AAAA |
| ATOM | 1470 | CB | PHE A | 186 | 28.513 | 19.937 | 67.164 | 1.00 | | |
| ATOM | 1471 | CG | PHE A | | 27.057 | 20.037 | | | | AAAA |
| | | | | | | | 67.500 | 1.00 | | AAAA |
| MOTA | 1472 | | PHE A | | 26.359 | 18.918 | | 1.00 | 17.70 | AAAA |
| MOTA | 1473 | CD2 | PHE A | 186 | 26.358 | 21.213 | 67.263 | 1.00 | 17.46 | AAAA |
| MOTA | 1474 | CE1 | PHE A | 186 | 24.999 | 18.964 | 68.147 | 1.00 | | |
| MOTA | 1475 | | PHE A | | 24.997 | 21.271 | | | | AAAA |
| | | | | | | | 67.459 | 1.00 | | AAAA |
| MOTA | 1476 | CZ | PHE A | | | 20.138 | 67.905 | 1.00 | | AAAA |
| ATOM | 1477 | С | PHE A | 186 | 28.464 | 20.911 | 64.895 | 1.00 | 19.18 | AAAA |
| MOTA | 1478 | 0 | PHE A | 186 | 29.079 | 21.940 | 65.129 | 1.00 | | AAAA |
| MOTA | 1479 | N | VAL A | 187 | 27.520 | 20.834 | 63.964 | | | |
| ATOM | 1480 | CA | VAL A | | | | | 1.00 | | AAAA |
| | | | | | 27.137 | 21.993 | 63.160 | 1.00 | | AAAA |
| ATOM | 1481 | CB | VAL A | | 27.006 | 21.630 | 61.655 | 1.00 | 14.30 | AAAA |
| ATOM | 1482 | CG1 | VAL A | 187 | 26.628 | 22.869 | 60.828 | 1.00 | 10.34 | AAAA |
| ATOM | 1483 | CG2 | VAL A | 187 | 28.314 | 21.031 | 61.160 | 1.00 | | AAAA |
| MOTA | 1484 | C | VAL A | | 25.806 | | | | | |
| | | | | | | 22.511 | 63.665 | 1.00 | | AAAA |
| ATOM | 1485 | 0 | VAL A | | 24.852 | 21.746 | 63.792 | 1.00 | 16.95 | AAAA |
| ATOM. | 1486 | N · | LEU A | 188 | 25.763 | 23.809 | 63.960 | 1.00 | 18.66 | AAAA |
| MOTA | 1487 | CA | LEU A | 188 | 24.555 | 24.507 | 64.460 | 1.00 | | AAAA |
| ATOM | 1488 | CB | LEU A | | 24.752 | 24.995 | 65.914 | 1.00 | | |
| ATOM | 1489 | CG | LEU A | | | | | | | AAAA |
| | | | | | 23.702 | 26.019 | 66.395 | 1.00 | | AAAA |
| ATOM | 1490 | | LEU A | | 22.365 | 25.323 | 66.493 | 1.00 | 19.77 | AAAA |
| ATOM | 1491 | CD2 | LEU A | 188 | 24.085 | 26.627 | 67.750 | 1.00 | 20.63 | AAAA |
| ATOM | 1492 | С | LEU A | 188 | 24.297 | 25.735 | 63.591 | 1.00 | | AAAA |
| ATOM | 1493 | o | LEU A | | 25.223 | | | | | |
| | | | | | | 26.484 | 63.288 | 1.00 | | AAAA |
| MOTA | 1494 | N | SER A | | 23.049 | 25.987 | 63.233 | 1.00 | 19.32 | AAAA |
| MOTA | 1495 | CA | SER A | 189 | 22.786 | 27.130 | 62.381 | 1.00 | 18.06 | AAAA |
| ATOM | 1496 | CB | SER A | 189 | 22.970 | 26.715 | 60.906 | 1.00 | | AAAA |
| ATOM | 1497 | OG | SER A J | | 22.559 | 27.731 | 59.998 | 1.00 | | |
| | 1498 | Č | | | | _ | | | | AAAA |
| MO7 A | | | SER A I | | 21.418 | 27.751 | 62.554 | 1.00 | | AAAA |
| MO'1 K | 1499 | 0 | SER A] | 189 | 20.404 | 27.051 | 62.540 | 1.00 | 19.54 | AAAA |
| A_OM | 1500 | N | LEU A 1 | 190 | 21.386 | 29.067 | 62.722 | 1.00 | 16.97 | AAAA |
| ATOM | 1501 | CA | LEU A 1 | 190 | 20.117 | 29.772 | 62.797 | 1.00 | | |
| ATOM | 1502 | CB | LEU A 1 | - | 20.097 | 30.865 | | | | AAAA |
| | | | | | | | 63.886 | 1.00 | | AAAA |
| ATOM | 1503 | | LEU A 1 | | 20.534 | 30.600 | 65.337 | 1.00 | | AAAA |
| ATOM | 1504 | CD1 | LEU A 1 | 190 | 19.643 | 31.406 | 66.266 | 1.00 | 15.50 | AAAA |
| ATOM | 1505 | CD2 | LEU A 1 | 90 | 20.455 | 29.147 | 65.686 | 1.00 | 5 15 | AAAA |
| ATOM | 1506 | | LEU A 1 | | 20.111 | 30.408 | 61.416 | | | |
| | | | | | | | | 1.00 1 | | AAAA |
| ATOM | 1507 | | LEU A 1 | | 21.136 | 30.891 | 60.967 | 1.00 | | AAAA |
| MOTA | 1508 | N | HIS A 1 | .91 | 18.975 | 30.397 | 60.736 | 1.00 2 | 21.75 | AAAA |
| MOTA | 1509 | CA | HIS A 1 | .91 | 18.897 | 30.955 | 59.383 | 1.00 2 | | AAAA |
| ATOM | 1510 | | HIS A 1 | | 19.626 | 30.013 | 58.426 | | | |
| | | | | | | | | 1.00 2 | | AAAA |
| MOTA | 1511 | | HIS A 1 | | 19.157 | 28.597 | 58.533 | 1.00 2 | 4.26 | AAAA |
| ATOM | 1512 | | HIS A 1 | | 19.770 | 27.485 | 59.009 | 1.00 2 | 23.78 | AAAA |
| MOTA | 1513 | ND1 | HIS A 1 | .91 | 17.869 | 28.217 | 58.217 | 1.00 2 | | AAAA |
| ATOM | 1514 | | HIS A 1 | | 17.709 | 26.935 | 58.491 | 1.00 2 | | |
| | | | | | | • | | | | AAAA |
| ATOM | 1515 | | HIS A 1 | | 18.849 | 26.467 | 58.973 | 1.00 2 | | AAAA |
| MOTA | 1516 | | HIS A 1 | | 17.446 | 31.119 | 58.926 | 1.00 2 | 4.10 | AAAA |
| ATOM | 1517 | 0 | HIS A 1 | .91 | 16.519 | 30.658 | 59.596 | 1.00 2 | | AAAA |
| MOTA | 1518 | | GLN A 1 | | 17.249 | 31.789 | 57.794 | 1.00 2 | | AAAA |
| | 1310 | ٠. ' | | | | 52.705 | | 1.00 2 | | www |

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Figure 19-24

| | | | | | | ~ | | | | | | |
|--------------|----------------|-----------|----------------|---|------------|------------------|------------------|------------------|------|----------------|---|--------------|
| MOTA | 1519 | CA | GLN | A | 192 | 15.899 | 31.959 | 57.269 | 1.00 | 25.77 | | AAAA |
| ATOM | 1520 | CB | GĪN | Α | 192 | 15.881 | 32.896 | 56.060 | | 26.51 | | AAAA |
| ATOM | 1521 | CG | GLN | Α | 192 | 16.467 | 34.271 | 56.325 | | 26.99 | | AAAA |
| ATOM | 1522 | CD | | | 192 | 16.581 | 35.076 | 55.062 | 1.00 | 27.98 | | AAAA |
| ATOM | 1523 | | GLN | | | 15.583 | 35.496 | 54.493 | 1.00 | 30.48 | | AAAA |
| MOTA | 1524 | NE2 | | | | 17.802 | 35.274 | 54.595 | 1.00 | 29.04 | | AAAA |
| ATOM | 1525 | C | | | 192 | 15.463 | 30.573 | 56.832 | | 25.77 | | AAAA |
| MOTA | 1526 | 0 | | | 192 | 16.211 | 29.865 | 56.169 | | 26.73 | | AAAA |
| MOTA | 1527 | N | | | 193 | 14.259 | 30.184 | 57.214 | | 25.48 | | AAAA |
| MOTA | 1528 | CA | | | 193 | 13.750 | 28.877 | 56.863 | | 24.51 | | AAAA |
| ATOM | 1529 1530 | CB OG | | | 193 | 12.288 | 28.788 | 57.286 | | 23.77 | | AAAA |
| MOTA MOTA | 1531 | C | | | 193 193 | 11.753 13.906 | 27.517 | 57.010 | | 24.81 | | AAAA |
| ATOM | 1532 | õ | | | 193 | 13.736 | 28.597 29.479 | 55.361 54.522 | | 24.53 | | AAAA |
| ATOM | 1533 | N | | | 194 | 14.226 | 27.348 | 55.007 | | 22.32 25.69 | | AAAA |
| ATOM | 1534 | CD | | | 194 | 14.411 | 26.167 | 55.862 | | 25.02 | | AAAA AAAA |
| ATOM | 1535 | CA | | | 194 | 14.399 | 26,976 | 53.604 | | 27.05 | | AAAA |
| ATOM | 1536 | CB | PRO | | | 14.906 | 25.535 | 53.697 | | 26.30 | | AAAA |
| MOTA | 1537 | CG | PRO | A | 194 | 15.479 | 25.466 | 55.124 | | 26.44 | | AAAA |
| MOTA | 1538 | С | PRO | Α | 194 | 13.076 | 27.057 | 52.849 | | 27.79 | | AAAA |
| MOTA | 1539 | 0 | PRO | А | 194 | 13.066 | 27.057 | 51.625 | 1.00 | 28.82 | * | AAAA |
| MOTA | 1540 | N | GLU | | | 11.966 | 27.133 | 53.582 | | 28.29 | | AAAA |
| MOTA | 1541 | CA | GLU | | | 10.656 | 27.187 | 52.950 | | 29.08 | | AAAA |
| MOTA | 1542 | CB | GLU | | | 9.534 | 27.030 | 54.001 | | 31.08 | | AAAA |
| ATOM | 1543 | CG | GLU | | | 9.070 | 28.294 | 54.722 | | 35.07 | | AAAA |
| ATOM ATOM | 1544 . 1545 | CD | GLU | | | 7.850 | 28.980 | 54.064 | | 38.05 | | AAAA |
| ATOM | 1545 | | GLU | | | 7.389 7.342 | 30.017 28.487 | 54.601 53.024 | | 38.80 | | AAAA |
| ATOM | 1547 | C | GLU | | | 10.483 | 28.471 | 52.150 | | 39.20 28.05 | | AAAA |
| ATOM | 1548 | ō | GLU | | | 9.722 | 28.512 | 51.189 | | 28.57 | | AAAA AAAA |
| ATOM | 1549 | N | TYR | | - | 11.223 | 29.510 | 52.514 | | 27.39 | | AAAA |
| ATOM | 1550 | CA | TYR | | | 11.108 | 30.769 | 51.802 | | 25.80 | | AAAA |
| MOTA | 1551 | CB | TYR | А | 196 | 10.275 | 31.743 | 52.645 | | 24.97 | | AAAA |
| MOTA | 1552 | CG | TYR | | | 10.971 | 32.281 | 53.868 | 1.00 | 23.41 | | AAAA |
| MOTA | 1553 | | TYR | | | 11.911 | 33.306 | 53.765 | | 23.99 | | AAAA |
| ATOM | 1554 | | TYR | | | 12.559 | 33.805 | 54.892 | | 23.44 | | AAAA |
| MOTA | 1555 | CD2 | TYR | | | 10.697 | 31.768 | 55.126 | | 23.24 | | AAAA |
| ATOM | 1556 1557 | CE2 | TYR | | | 11.336 | 32.256 | 56.254 | | 23.93 | | AAAA |
| ATOM ATOM | 1558 | OH | TYR | | | 12.265 12.913 | 33.270 33.731 | 56.133 57.247 | | 24.07 25.06 | | AAAA |
| ATOM | 1559 | C | TYR | | | 12.450 | 31.406 | 51.411 | | 24.97 | | AAAA AAAA |
| ATOM | 1560 | ō | TYR | | | 12.475 | 32.495 | 50.840 | | 25.14 | | AAAA |
| ATOM | 1561 | N | ALA | | | 13.563 | 30.737 | 51.686 | | 23.81 | | AAAA |
| ATOM | 1562 | CA | ALA | А | 197 | 14.855 | 31.330 | 51.337 | | 23.32 | | AAAA |
| MOTA | 1563 | CB | ALA | A | 197 | 15.350 | 32.220 | 52.488 | 1.00 | 23.33 | | AAAA |
| ATOM - | 1564 | С | ALA | | | 15.952 | 30.356 | 50.957 | | 22.74 | | AAAA |
| MOTA | 1565 | | ALA | | | 15.951 | 29.207 | .51 . 37 ' | | 22.47 | | AAAA |
| ATOM · | 1566 | | PHE | | | 16,900 | 30.852 | 50.16 | 1.00 | 23.23 | | AAAA |
| ATOM | 1567 | CA | PHE | | - | 18.062 | 30.081 | 49.741 | | 23.68 | | AAAA |
| ATOM | 1568 | CB | PHE | | | 19.083 | 31.006 | 49.069 | | 23.33 | | AAAA |
| ATOM ATOM | 1569 1570 | CG CD1 | PHE | | | 20.250 20.151 | 30.280 29.713 | 48.464 47.203 | | 22.75 | | AAAA |
| ATOM | 1571 | | PHE | | | 21.436 | 30.127 | 49.175 | 1.00 | 23.32 | | AAAA AAAA |
| MOTA | 1572 | | PHE | | | 21.207 | 29.003 | 46.645 | | 22.13 | | AAAA |
| ATOM | 1573 | | PHE | | | 22.512 | 29.408 | 48.622 | | 22.83 | | AAAA |
| ATOM | 1574 | CZ | PHE | A | 198 | 22.386 | 28.849 | 47.351 | | 22.55 | | AAAA |
| ATOM | 1575 | С | PHE | A | 198 | 18.689 | 29.490 | 51.008 | 1.00 | 23.69 | | AAAA |
| ATOM | 1576 | 0 | PHE . | A | 198 | 18.802 | 30.171 | 52.012 | | 22.85 | | AAAA |
| MOTA | 1577 | N | PRO | | | 19.166 | 28.236 | 50.954 | 1.00 | 23.96 | | AAAA |
| MOTA | 1578 | CD | PRO | | | 19.833 | 27.639 | 52.123 | | 24.26 | | AAAA |
| ATOM | 1579 | CA | PRO | | | 19.199 | 27.286 | 49.837 | | 24.70 | | AAAA |
| ATOM | 1580 | CB | PRO . | | | 20.163 | 26.222 | 50.357 | | 23.30 | | AAAA |
| ATOM | 1581 | | PRO | | | 19.797 | 26.162 | 51.782 | | 23.21 | | AAAA |
| ATOM | 1582 | C | PRO . | | | 17.885 | 26.679 | 49.326 | | 25.22 | | AAAA |
| ATOM | 1583 | | PRO . PHE . | | | 17.866 | 26.145 | 48.215 | | 26.24 | | AAAA |
| ATCM | 1584 | N | rac. | ~ | £ 00 | 16.811 | 26.756 | 50.116 | 1.00 | 25.09 | | AAAA |

SUBSTITUTE SHEET (RULE 26)

| | | | | | • | | | | | |
|--------|------|-----|----------------|-------|---|--------|---------|---------|------------------------|--------|
| 3.0034 | 1505 | CA | PHE A | 200 | | 15.497 | 26.190 | 49.763 | 1.00 26.2 9 | AAAA |
| MOTA | 1585 | | | | | | 26.567 | 48.340 | 1.00 25.65 | AAAA |
| ATOM | 1586 | CB | PHE A | 200 | | 15.064 | | | | |
| ATOM | 1587 | CG | PHE A | 200 | | 14.863 | 28.035 | 48.122 | 1.00 24.65 | AAAA |
| | 1588 | CDI | PHE A | | | 15.806 | 28.781 | 47.439 | 1.00 24.42 | AAAA |
| ATOM | | | | | | | 28.671 | 48.608 | 1.00 23.79 | AAAA |
| MOTA | 1589 | | PHE A | | | 13.735 | | | | |
| ATOM_ | 1590 | CE1 | PHE A | 200. | | 15.631 | 30.125 | 47.246 | 1.00 24.41 | AAAA |
| | 1591 | | PHE A | | | 13.552 | 30.035 | 48.418 | 1.00 24.94 | AAAA |
| MOTA | | | | | | | 30.760 | 47.738 | 1.00 24.57 | AAAA |
| MOTA | 1592 | CZ | PHE A | 200 | | 14.499 | | | | |
| MOTA | 1593 | С | PHE A | 200 | | 15.415 | 24.656 | 49.863 | 1.00 28.54 | AAAA |
| - | 1594 | 0 | PHE A | | | 14.386 | 24.096 | 50.251 | 1.00 28.76 | AAAA |
| MOTA | | | | | | | | 49.504 | 1.00 29.67 | AAAA |
| MOTA | 1595 | N | GLU A | | | 16.499 | | | | |
| MOTA | 1596 | CA | GLU A | 201 | | 16.539 | 22.528 | 49.524 | 1.00 31.88 | AAAA |
| | 1597 | CB | GLU A | 201 | - | 17.434 | 22.045 | 48.392- | 1.00 32.71 | AAAA |
| MOTA | | | | | | 16.897 | | 47.017 | 1.00 34.87 | AAAA |
| MOTA | 1598 | CG | GLU A | | | | | | | |
| MOTA | 1599 | CD | GLU A | 201 | | 17.898 | 22.147 | | 1.00 35.14 | AAAA |
| MOTA | 1600 | OE1 | GLU A GLU A | 201 | | 18.299 | 20.982 | 45.735 | 1.00 36.09 | - AAAA |
| - | - | 022 | CTIL | 201 | | 19 296 | .23.112 | 45.221 | 1.00 36.30 | AAAA |
| ATOM | 1601 | | | | | 16.200 | | | 1 00 33 77 | |
| MOTA | 1602 | С | GLU A | | | 16.997 | 21.894 | | 1.00 32.77 | AAAA |
| ATOM | 1603 | 0 | GLU A | 201 | | 16.806 | 20.690 | 51.046 | 1.00 33.44 | AAAA |
| | | | LYS A | | | 17.599 | 22.690 | 51.711 | 1.00 32.31 | AAAA |
| MOTA | 1604 | N | | | | | | 52.974 | 1.00 32.09 | AAAA |
| MOTA | 1605 | CA | LYS A | | | 18.101 | | | 1.00 32.09 | AAAA |
| MOTA | 1606 | CB | LYS A | 202 | | 19.565 | 21.750 | 52.811 | 1.00 33.02 | AAAA |
| | 1607 | CG | LYS A | | | 19.836 | 20.847 | 51.623 | 1.00 34.95 | AAAA |
| MOTA | | | | | | 21.334 | 20.619 | | 1.00 37.92 | AAAA |
| ATOM | 1608 | CD | LYS A | | | | | | | |
| MOTA | 1609 | CE | LYS A | 202 | | 21.655 | 19.804 | | 1.00 39.19 | AAAA |
| | 1610 | NZ | LYS A | 202 | | 23.120 | 19.522 | 49.988 | 1.00 38.58 | AAAA |
| MOTA | | | | | | 17.995 | | 54.037 | 1.00 30.85 | AAAA |
| MOTA | 1611 | С | LYS A | | | | | | | |
| MOTA | 1612 | 0 | LYS A | 202 | | 17.706 | 24.389 | 53.739 | 1.00 30.49 | AAAA |
| MOTA | 1613 | N | GLY A | 203 | | 18.238 | 22.867 | 55.281 | 1.00 30.81 | AAAA |
| | | CA | GLY A | | | 18.159 | 23.831 | 56.356 | 1.00 30.86 | AAAA |
| MOTA | 1614 | | | | | | | 57.280 | 1.00 30.84 | AAAA |
| MOTA | 1615 | С | GLY A | | | 16.991 | | | | |
| MOTA | 1616 | 0 | GLY A | 203 | | 16.828 | 24.285 | | 1.00 31.58 | |
| MOTA | 1617 | И | PHE A | 204 | | 16.182 | 22.570 | 56.965 | 1.00 30.54 | AAAA |
| | | | PHE A | | | 15.025 | 22.241 | 57.797 | 1.00 30.51 | AAAA |
| ATOM | 1618 | CA | • | | | | | | 1.00 29.06 | AAAA |
| ATOM | 1619 | CB | PHE A | 204 | | 14.061 | 21.317 | 37.036 | | |
| ATOM | 1620 | CG | PHE A | 204 | | 13.524 | 21.890 | 55.787 | | AAAA |
| ATOM | 1621 | CD1 | PHE A | 204 | | 14.222 | 21.762 | 54.601 | 1.00 26.52 | AAAA |
| | | | PHE A | | | 12.307 | 22.548 | 55.779 | 1.00 26.50 | AAAA |
| ATOM | 1622 | | | | | | | | 1.00 26.44 | AAAA |
| MOTA | 1623 | CEl | PHE A | 204 | | 13.713 | 22.276 | | | |
| ATOM | 1624 | CE2 | PHE A | 204 | | 11.786 | 23.069 | 54.600 | 1.00 26.69 | AAAA |
| | 1625 | CZ | PHE A | | | 12.490 | 22.931 | 53.416 | 1.00 25.65 | AAAA |
| MOTA | | | | | | | 21.590 | 59.127 | 1.00 30.87 | AAAA |
| atom | 1626 | С | PHE A | | | 15.401 | | | | AAAA |
| MOTA | 1627 | 0 | PHE A | 204 | | 16.395 | 20.875 | 59.228 | 1.00 31.12 | |
| ATOM | 1628 | N | LEU A | 205 | | 14.580 | 21.844 | 60.139 | 1.00 31.22 | AAAA |
| | 1629 | CA | LEU A | | | 14.782 | 21.329 | 61.489 | 1.00 31.43 | AAAA |
| MOTA | | | | | | 13.575 | 21.691 | | | AAAA |
| ATOM | 1630 | CB | LEU A | | | | | | | |
| ATOM | 1631 | CG | LEU A | : 235 | | 13.603 | 21.078 | | 1.00 31.76 | AAAA |
| ATOM | 1632 | CD1 | LEU A | 2.15 | | 14.894 | 21.492 | 64.457 | 1.00 32.36 | AAAA |
| | | | LEU A | | | 12.379 | 21.516 | 64.536 | 1.00 31.31 | AAAA |
| MOTA | 1633 | | | | | | | 61.625 | 1.00 31.35 | AAAA |
| ATOM | 1634 | С | LEU A | | | 15.026 | 19.829 | | | |
| MOTA | 1635 | 0 | LEU A | 205 | | 15.714 | 19.392 | 62.546 | 1.00 31.40 | AAAA |
| | 1636 | N | GLU A | | | 14.448 | 19.059 | 60.707 | 1.00 31.79 | AAAA |
| ATOM | | | | | | 14.509 | 17.603 | 60.706 | 1.00 32.08 | AAAA |
| ATOM | 1637 | CA | GLU A | | | | | | | |
| MOTA | 1638 | ÇВ | GLU A | 206 | | 13.485 | 17.054 | 59.716 | 1.00 33.18 | AAAA |
| ATOM | 1639 | ĊG | GLU A | 206 | | 12,069 | 17.651 | 59.829 | 1.00 34.20 | AAAA |
| | | | | | | 11,973 | 19.136 | 59.453 | 1.00 33.44 | AAAA |
| ATOM | 1640 | CD | GLU A | | | | | 59.422 | 1.00 33.32 | AAAA |
| ATOM | 1641 | | GLU A | | | 10.854 | 19.675 | • | | |
| ATOM | 1642 | OE2 | GLU A | 206 | | 13.005 | 19.777 | 59.194 | 1.00 35.12 | AAAA |
| | 1643 | c | GLU A | | | 15.882 | 17.045 | 60.363 | 1.00 32.34 | AAAA |
| ATOM | | | | | | | 15.909 | 60.706 | 1.00 31.83 | AAAA |
| MOTA | 1644 | 0 | GLU A | | | 16.209 | | | | |
| MOTA | 1645 | N | GLU A | 207 | | 16.680 | 17.847 | 59.670 | 1.00 32.48 | AAAA |
| | 1646 | CA | GLU A | | | 18.017 | 17.431 | 59.287 | 1.00 31.67 | AAAA |
| MOTA | | | | | | 18.552 | 18.385 | 58.238 | 1.00 30.39 | AAAA |
| MOTA | 1647 | CB | GLU A | | | | | | | AAAA |
| MOTA | 1648 | CG | GLU A | 207 | | 17.768 | 18.316 | 56.960 | 1.00 29.63 | |
| ATOM | 1649 | CD | GLU A | 207 | | 17.953 | 19.547 | 56.121 | 1.00 30.04 | AAAA |
| | | | GLU A | | | 19,108 | 19.991 | 55.971 | 1.00 30.31 | AAAA |
| ATOM | 1650 | OFT | GDO W | 201 | | 22.200 | | | | |

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| ATOM | 1651 | OE2 | GLU | A | 207 | 16.947 | 20.070 | 55.604 | 1.00 30.76 | AAAA |
|------|------|-----|-----|---|-----|--------|--------|--------|------------|--------|
| ATOM | 1652 | С | GLU | A | 207 | 18.879 | 17.433 | 60.537 | 1.00 32.04 | AAAA |
| ATOM | 1653 | 0 | | | 207 | 19.472 | 18.448 | 60.910 | 1.00 31.57 | AAAA |
| ATOM | 1654 | N | | | 208 | 18.935 | 16.272 | 61.178 | 1.00 32.57 | AAAA |
| ATOM | 1655 | CA | | | 208 | 19.674 | 16.111 | 62.408 | 1.00 33.37 | AAAA |
| ATOM | 1656 | CB | | | 208 | 18.709 | 15.647 | 63.519 | 1.00 33.65 | AAAA |
| | 1657 | | ILE | | | 19,443 | 15.380 | 64.806 | 1.00 34.11 | AAAA |
| ATOM | | | | | | | | 63.757 | 1.00 33.94 | |
| MOTA | 1658 | | ILE | | | 17.673 | 16.742 | | | AAAA |
| ATOM | 1659 | | ILE | | | 16.628 | 16.386 | 64.794 | 1.00 37.00 | AAAA |
| MOTA | 1660 | C | | | 208 | 20.863 | 15.174 | 62.280 | 1.00 34.00 | AAAA |
| ATOM | 1661 | 0 | | | 208 | 21.506 | 14.829 | 63.265 | 1.00 34.40 | AAAA |
| MOTA | 1662 | N | GLY | A | 209 | 21.177 | 14.768 | 61.062 | 1.00 34.64 | AAAA |
| MOTA | 1663 | CA | GLY | A | 209 | 22.321 | 13.903 | 60.913 | 1.00 35.55 | AAAA · |
| MOTA | 1664 | С | GLY | A | 209 | 22.164 | 12.671 | 60.057 | 1.00 36.80 | AAAA |
| ATOM | 1665 | 0 | GLY | Α | 209 | 21.148 | 12.461 | 59.400 | 1.00 37.32 | AAAA |
| MOTA | 1666 | N | GLU | Α | 210 | 23.199 | 11.836 | 60.100 | 1.00 37.78 | AAAA |
| ATOM | 1667 | CA | GLU | А | 210 | 23.256 | 10.621 | 59.315 | 1.00 38.04 | AAAA |
| ATOM | 1668 | CB | GLU | A | 210 | 23.600 | 11.013 | 57.892 | 1.00 38.54 | AAAA |
| ATOM | 1669 | CG | | | 210 | 23.469 | 9.960 | 56.858 | 1.00 38.99 | AAAA |
| ATOM | 1670 | CD | | | 210 | 24.118 | 10.412 | 55.580 | 1.00 40.10 | AAAA |
| ATOM | 1671 | | GLU | | | 25.365 | 10.437 | 55.555 | 1.00 40.86 | AAAA |
| ATOM | 1672 | OE2 | GLU | | | 23.396 | 10.767 | 54.619 | 1.00 40.41 | AAAA |
| | 1673 | C | | | 210 | 24.377 | 9.770 | 59.894 | 1.00 37.98 | AAAA |
| MOTA | | ō | | | 210 | 25.498 | 10.244 | 60.041 | 1.00 38.52 | AAAA |
| ATOM | 1674 | | | | | | 8.517 | 60.220 | 1.00 38.02 | |
| MOTA | 1675 | N | | | 211 | 24.085 | | 60.770 | 1.00 38.02 | AAAA |
| ATOM | 1676 | CA | | | 211 | 25.116 | 7.654 | | | AAAA |
| ATOM | 1677 | C | | | 211 | 25.542 | 8.075 | 62.164 | 1.00 38.26 | AAAA |
| ATOM | 1678 | 0 | | | 211 | 24.697 | 8.443 | 62.977 | 1.00 37.82 | AAAA |
| ATOM | 1679 | N | | | 212 | 26.848 | 8.030 | 62.434 | 1.00 38.20 | AAAA |
| MOTA | 1680 | CA | | | 212 | 27.396 | 8.399 | 63.743 | 1.00 37.56 | AAAA |
| MOTA | 1681 | CB | | | 212 | 28.921 | 8.209 | 63.766 | 1.00 38.86 | AAAA |
| ATOM | 1682 | CG | | | 212 | 29.416 | 6.810 | 63.385 | 1.00 40.93 | AAAA |
| MOTA | 1683 | CD | | | 212 | 29.001 | 5.746 | 64.405 | 1.00 42.04 | AAAA |
| MOTA | 1684 | CE | | | 212 | 29.251 | 4.318 | 63.891 | 1.00 42.80 | AAAA |
| ATOM | 1685 | NZ | | | 212 | 30.673 | 4.002 | 63.562 | 1.00 42.32 | AAAA |
| MOTA | 1686 | С | | | 212 | 27.093 | 9.859 | 64.054 | 1.00 37.08 | AAAA |
| ATOM | 1687 | 0 | LYS | A | 212 | 27.075 | 10.269 | 65.218 | 1.00 36.94 | AAAA |
| MOTA | 1688 | N | GLY | Æ | 213 | 26.854 | 10.636 | 63.002 | 1.00 35.41 | AAAA |
| MOTA | 1689 | CA | ĢLY | A | 213 | 26.592 | 12.054 | 63.170 | 1.00 34.24 | AAAA |
| ATOM | 1690 | С | GLY | A | 213 | 25.163 | 12.438 | 63.470 | 1.00 33.27 | AAAA |
| ATOM | 1691 | 0 | GLY | A | 213 | 24.861 | 13.611 | 63.666 | 1,00 33.29 | AAAA |
| ATOM | 1692 | N | LYS | A | 214 | 24.280 | 11.451 | 63.512 | 1.00 31.79 | AAAA |
| ATOM | 1693 | CA | LYS | A | 214 | 22.883 | 11.710 | 63.794 | 1.00 30.47 | AAAA |
| MOTA | 1694 | CB | LYS | A | 214 | 22.111 | 10.396 | 63.737 | 1.00 30.35 | AAAA |
| ATOM | 1695 | CG | LYS | A | 214 | 20.676 | 10.552 | 63.280 | 1.00 30.45 | AAAA |
| ATOM | 1696 | CD | LYS | A | 214 | 20.141 | 9.241 | 62.759 | 1.00 29.75 | AAAA |
| ATOM | 1697 | CE | LYS | A | 214 | 18.737 | 9.400 | 62.229 | 1.00 30.19 | AAAA |
| ATOM | 1698 | NZ | LYS | Α | 214 | 18.179 | 8.138 | 61.671 | 1.00 31.35 | AAAA |
| ATOM | 1699 | С | LYS | | | 22.778 | 12.374 | 65.168 | 1.00 30.31 | AAAA |
| ATOM | 1700 | 0 | | | 214 | 23.193 | 11.814 | 66.177 | 1.00 30.44 | AAAA |
| MOTA | 1701 | N | | | 215 | 22.243 | 13.590 | 65.192 | 1.00 29.95 | AAAA |
| ATOM | 1702 | CA | GLY | | | 22.128 | 14.325 | 66.437 | 1.00 29.16 | AAAA |
| ATOM | 1703 | c | GLY | | | 23.222 | 15.379 | 66.582 | 1.00 28.54 | AAAA |
| ATOM | 1704 | õ | GLY | | | 23.306 | 16.061 | 67.602 | 1.00 28.27 | AAAA |
| | 1705 | Ŋ | | | 216 | 24.063 | 15.521 | 65.561 | 1.00 27.35 | AAAA |
| MOTA | | • | | | 216 | 25.150 | 16.497 | 65.616 | 1.00 27.08 | AAAA |
| ATOM | 1706 | CA | | | | | | 65.531 | 1.00 28.38 | AAAA |
| MOTA | 1707 | CB | | | 216 | 26.516 | 15.800 | 66.757 | 1.00 30.21 | AAAA |
| ATOM | 1708 | CG | | | 216 | 26.786 | 14.966 | 66.955 | | AAAA |
| atom | 1709 | | TYR | | | 26.138 | 13.735 | | 1.00 29.81 | |
| ATOM | 1710 | CE1 | TYR | | | 26.311 | 13.014 | 68.138 | 1.00 30.03 | AAAA |
| ATOM | 1711 | | TYR | | | 27.619 | 15.450 | 67.774 | 1.00 29.71 | AAAA |
| ATOM | 1712 | CE2 | TYR | | | 27.798 | 14.741 | 68.957 | 1.00 29.96 | AAAA |
| MCTA | 1713 | CZ | | | 216 | 27.143 | 13.528 | 69.138 | 1.00 30.84 | AAAA |
| ATCM | 1714 | OH | | | 216 | 27.297 | 12.859 | 70.332 | 1.00 31.14 | AAAA |
| MOTA | 1715 | С | | | 216 | 25.055 | 17.599 | 64.581 | 1.00 25.40 | AAAA |
| ATOM | 1716 | 0 | TYR | A | 216 | 26.046 | 18.240 | 64.243 | 1.00 26.38 | AAAA |

| | | | | ~ | 07 045 | | CA 07C | 1 00 00 55 | |
|--------|-------|-------|---------|-------|----------|--------|--------|------------|-------|
| ATOM | 1717 | N | ASN A | 21/ | 23.845 | 17.791 | 64.076 | 1.00 23.55 | AAAA |
| MOTA | 1718 | CA | ASN A | 217 | 23.549 | 18.830 | 63.119 | 1.00 21.52 | AAAA |
| | 1719 | CB | ASN A | 217 | 23.431 | 18.282 | 61.699 | 1.00 20.64 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 1720 | CG | asn a | | 23.202 | 19.386 | 60.669 | 1.00 20.29 | AAAA |
| MOTA | 1721 | OD1 | . ASN A | 217 | 22.089 | 19.888 | 60.499 | 1.00 18.03 | AAAA |
| ATOM | 1722 | אדוי2 | ASN A | 217 | 24.274 | 19.790 | 60.004 | 1.00 19.95 | AAAA |
| | | | | | | | | 1.00 21.64 | |
| ATOM | 1723 | C | asn a | | 22.216 | 19.346 | 63.605 | | AAAA |
| MOTA | 1724 | 0 | ASN A | 217 | 21.263 | 18.576 | 63.757 | 1.00 20.34 | AAAA |
| ATOM | 1725 | N | LEU A | 218 | 22.165 | 20.647 | 63.873 | 1.00 22.22 | AAAA |
| | | | LEU A | | 20.960 | 21.282 | 64.388 | 1.00 22.03 | AAAA |
| MOTA | 1726 | CA | | | | | | | |
| MOTA | 1727 | CB | LEU A | 218 | 21.195 | 21.711 | 65.840 | 1.00 20.97 | AAAA |
| ATOM | 1728 | CG | LEU A | 218 | 20.051 | 21.838 | 66.841 | 1.00 20.94 | AAAA |
| | 1729 | _ | LEU A | | 20.513 | 22.744 | 67.936 | 1.00 20.31 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 1730 | CDZ | LEU A | | 18.818 | 22.412 | 66.227 | 1.00 21.27 | AAAA |
| MOTA | 1731 | С | LEU A | 218 | 20.669 | 22.513 | 63.547 | 1.00 22.70 | AAAA |
| ATOM | 1732 | 0 | LEU A | 218 | 21.451 | 23.454 | 63.557 | 1.00 22.64 | AAAA |
| | | | ASN A | | 19.564 | 22.491 | 62.808 | 1.00 24.00 | AAAA |
| MOTA | 1733 | И | | | | | | | |
| ATOM | 1734 | CA | asn a | 219 | 19.166 | 23.626 | | 1.00 25.33 | AAAA |
| MOTA | 1735 | CB | ASN A | 219 | 18.656 | 23.190 | 60.614 | 1.00 26.94 | AAAA |
| | 1736 | CG | ASN A | | 19.737 | 22.601 | 59.749 | 1.00 26.68 | AAAA |
| MOTA | | | | | | | 59.626 | 1.00 28.06 | |
| MOTA | 1737 | | ASN A | | 20.812 | 23.169 | | | AAAA |
| ATOM | 1738 | ND2 | . ASN A | 219 | 19.446 | 21.471 | 59.117 | 1.00 26.26 | AAAA |
| MOTA | 1739 | С | ASN A | 219 | 18.046 | 24.345 | 62.710 | 1.00 25.69 | AAAA |
| | 1740 | | ASN A | | 17.118 | 23.706 | 63.210 | 1.00 27.51 | AAAA |
| ATOM | | 0 | | | | | 62.753 | | |
| MOTA | 1741 | N | ILE A | | 18.122 | 25.667 | _ | 1.00 25.05 | AAAA |
| MOTA | 1742 | CA | ILE A | . 220 | 17.107 | 26.457 | 63.428 | 1.00 25.87 | AAAA |
| MOTA | 1743 | CB | ILE A | 220 | 17.733 | 27.331 | 64.557 | 1.00 25.04 | AAAA |
| | | CG2 | | _ | 16.654 | 28.152 | 65.227 | 1.00 25.24 | AAAA |
| MOTA | 1744 | | | | | | | | |
| ATOM | 1745 | CG1 | ILE A | 220 | 18.460 | 26.447 | 65.584 | 1.00 24.07 | AAAA |
| ATOM | 1746 | CD1 | ILE A | 220 | 17.557 | 25.502 | 66.378 | 1.00 22.28 | AAAA |
| ATOM | 1747 | С | ILE A | 220 | 16.430 | 27.370 | 62.414 | 1.00 26.20 | AAAA |
| | | ō | ILE A | | 16.801 | 28.534 | 62.265 | 1.00 25.35 | AAAA |
| MOTA | 1748 | | | | | | | | |
| MOTA | 1749 | N | PRO A | | 15,421 | 26.850 | 61.704 | 1.00 26.70 | AAAA |
| ATOM | 1750 | CD | PRO A | 221 | . 14.840 | 25.501 | 61.778 | 1.00 27.17 | AAAA |
| MOTA | 1751 | CA | PRO A | 221 | 14.706 | 27.640 | 60.703 | 1.00 27.67 | AAAA |
| | 1752 | CB | PRO A | | 13.771 | 26.613 | 60.064 | 1.00 26.81 | AAAA |
| ATOM | | | | | | | 60.346 | 1.00 27.36 | AAAA |
| MOTA | 1753 | CG | PRO A | | 14.473 | 25.293 | | | |
| ATOM | 1754 | С | PRO A | 221 | 13.944 | 28.763 | 61.390 | 1.00 28.61 | AAAA |
| ATOM | 1755 | 0 | PRO A | 221 | 13.218 | 28.515 | 62.363 | 1.00 29.91 | AAAA |
| | 1756 | N | LEU A | | 14.100 | 29.990 | 60.900 | 1.00 28.15 | AAAA |
| ATOM | | | | | | | | 1.00 28.48 | AAAA |
| MOTA | 1757 | CA | LEU A | | 13.408 | 31.117 | | | |
| ATOM | 1758 | CB | LEU A | 222 | 14.431 | 32.041 | 62.191 | 1.00 28.69 | AAAA |
| ATOM | 1759 | CG | LEU A | 222 | 15.187 | 31.394 | 63.371 | 1.00 28.67 | AAAA |
| | 1760 | | LEU A | | 16.304 | 32.300 | 63.837 | 1.00 28.62 | AAAA |
| ATOM | | | | | | | | 1.00 27.65 | ·AAAA |
| MOTA | 1761 | CD2 | LEU A | | 14.231 | 31.106 | 64.527 | | |
| ATOM | 1762 | C | LEU A | 222 | 12.726 | 31.882 | 60.518 | 1.00 28.44 | AAAA |
| ATOM | 1763 | 0 | LEU A | 222 | 12.318 | 31.958 | 59.325 | 1.00 27.90 | AAAA |
| | | | PRO A | | . 1113 | 32.441 | 61.009 | 1.00 28.79 | AAAA |
| ATOM | 1764 | N | | | | | | 1.00 29.20 | |
| ATOM | 1765 | CD | PRO A | | 10.966 | 32.357 | 62.410 | | AAAA |
| MOTA | 1766 | CA | PRO A | 223 | 10.437 | 33.202 | 60.227 | 1.00 29.36 | AAAA |
| ATOM | 1767 | CB | PRO A | 223 | 9.256 | 33.287 | 61.183 | 1.00 28.98 | AAAA |
| | | | PRO A | | 9.965 | 33.502 | 62.485 | 1.00 28.68 | AAAA |
| ATOM | 1768 | CG | | | | | | 1.00 30.15 | |
| MOTA | 1769 | С | PRO A | 223 | 10.890 | 34.585 | 59.753 | | AAAA |
| MOTA | 1770 | 0 | PRO A | 223 | 11.864 | 35.152 | 60.253 | 1.00 30.18 | AAAA |
| | 1771 | N | LYS A | 224 | 10.150 | 35.112 | 58.781 | 1.00 30.50 | AAAA |
| MOTA | | | LYS A | 224 | 10.398 | 36.422 | 58.213 | 1.00 29.92 | AAAA |
| MOTA | 1772 | CA | пто у | 224 | | | | | |
| MOTA | 1773 | CB | LYS A | 224 | 9.491 | 36.661 | 57.008 | 1.00 30.57 | AAAA |
| MOTA | 1774 | CG | LYS A | 224 | 9.588 | 35.676 | 55.893 | 1.00 30.06 | AAAA |
| | 1775 | CD | LYS A | 224 | 8.640 | 36.087 | 54.798 | 1.00 30.91 | AAAA |
| MOTA | | | 7 V C 7 | 224 | 8.575 | 35.051 | 53.705 | 1.00 32.15 | AAAA |
| MOTA | 1776 | CE | LYS A | | | | | | |
| MOTA | 1777 | NZ | LYS A | | 7.628 | 35.476 | 52.648 | 1.00 32.75 | AAAA |
| ATOM | 1778 | C | LYS A | 224 | 10.050 | 37.468 | 59.260 | 1.00 29.75 | AAAA |
| | 1779 | ō | LYS A | 224 | 9.308 | 37.193 | 60.196 | 1.00 29.84 | AAAA |
| ATOM | | | 711 A | 225 | 10.555 | 38.678 | 59.079 | 1.00 29.39 | AAAA |
| ATOM | 1780 | N | GLY A | 443 | | | | 1.00 29.87 | |
| MOTA | 1781 | CA | GLY A | 225 | 10.261 | 39.730 | 60.031 | | AAAA |
| ATOM | 1782 | C | GLY A | 225 | 10.809 | 39.447 | 61.415 | 1.00 29.85 | AAAA |
| TTOIT. | _, 00 | - | | | | | • . | | - |

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| ATOM | 1783 | 0 | GLY . | A 225 | 10.371 | 40.051 | 62.392 | 1.00 29.85 | AAAA |
|--------------|--------------|-------|-------|-------|------------------|-------------------|------------------|--------------------------|--------------|
| ATOM | 1784 | N | LEU . | A 226 | 11.775 | 38.536 | 61.499 | 1.00 29.50 | AAAA |
| ATOM | 1785 | CA | LEU . | A 226 | 12.374 | 38.175 | 62.778 | 1.00 29.80 | AAAA |
| ATOM | 1786 | CB | LEU . | A 226 | 13.513 | 37.170 | 62.570 | 1.00 28.81 | AAAA |
| ATOM | 1787 | CG | LEU . | A 226 | 14.097 | 36.514 | 63.820 | 1.00 27,29 | AAAA |
| ATOM | 1788 | | LEU / | | 13.132 | 35.452 | 64.275 | 1.00 26.06 | |
| ATOM | 1789 | . CD2 | LEU : | A 226 | 15.455 | 35.888 | 63.538 | 1.00 27.03 | AAAA |
| MOTA | 1790 | С | LEU / | A 226 | 12.936 | 39.428 | 63.448 | 1.00 30.68 | AAAA |
| MOTA | 1791 | 0 | LEU Z | A 226 | 13.636 | 40.217 | 62.804 | 1.00 30.57 | AAAA |
| ATOM | 1792 | N | ASN A | A 227 | 12.624 | 39.617 | 64.729 | 1.00 31.46 | AAAA |
| ATOM | 1793 | CA | ASN I | A 227 | _ 13.139 | 40.769 | 65.469 | 1.00 32.06 | AAAA |
| MOTA | 1794 | CB | ASN A | A 227 | 12.012 | 41.507 | 66.217 | 1.00 31.74 | AAAA |
| ATOM | 1795 | CG | ASN I | A 227 | 11.291 | 40.630 | 67.234 | 1.00 32.07 | AÀAA |
| MOTA | . 1796 | OD1 | ASN A | A 227 | 11.914 | 40.017 | 68.104 | 1.00 31.61 | AAAA |
| ATOM | 1797 | ND2 | ASN A | A 227 | 9.962 | 40.592 | 67.141 | 1.00 31.59 | AAAA |
| MOTA | 1798 | С | ASN A | A 227 | 14.225 | 40.334 | 66.444- | | AAAA |
| ATOM | 1799 | 0 | ASN A | A 227 | 14.413 | 39.140 | 66.688 | 1.00 32.78 | AAAA |
| MOTA | 1800 | N | ASP A | | 14.943 | 41.297 | 67.002 | 1.00 33.32 | AAAA |
| MOTA | 1801 | CA | ASP A | | 16.017 | 40.976 | 67.928 | 1.00 34.75 | AAAA |
| ATOM | 1802 | CB | ASP A | | 16.508 | 42.233 | 68.654 | 1.00 36.77 | AAAA |
| MOTA | 1803 | CG | | 1 228 | 17.154 | 43.238 | 67.714 | 1.00 37.28 | AAAA |
| MOTA | 1804 | | ASP A | | 17.662 | 42.816 | 66.652 | 1.00 37.78 | AAAA |
| MOTA | 1805 | | ASP A | | 17.180 | 44.443 | 68.054 | 1.00 37.21 | AAAA |
| MOTA | 1806 | C | ASP A | | 15.707 | 39.892 | 68.964 | 1.00 34.93 | AAAA |
| MOTA | 1807 | Ο. | ASP A | | 16.448 | 38.919 | 69.056 | 1.00 36.92 | AAAA |
| MOTA | 1808 | N | ASN A | | 14.635 | 40.054 | 69.741 | 1.00 33.90 | AAAA |
| MOTA | 1809 | CA | ASN A | | 14.268 | 39.079 | 70.775 | 1.00 33.01 | AAAA |
| ATOM | 1810 | CB | ASN A | | 12.965 | 39.481 | 71.455 | 1.00 33.79 | AAAA |
| MOTA | 1811 | CG | ASN A | | 13.131 | 40.663 | 72.369 | 1.00 34.04 | AAAA |
| ATOM - | 1812 | | ASN A | | 13.783 | 40.564 | 73.405 | 1.00 34.25 | AAAA |
| MOTA | 1813 1814 | C | ASN A | | 12.550 | 41.797 | 71.988 | 1.00 34.05 | AAAA |
| ATOM ATOM | 1815 | Ö | ASN A | | 14.114 14.529 | 37.656 | 70.276 | 1.00 32.98 | AAAA |
| ATOM | 1816 | Ŋ | GLU A | | 13.496 | 36.697. 37.523 | 70.944 69.108 | 1.00 32.77 1.00 32.02 | AAAA |
| ATOM | 1817 | CÀ | GLU A | | 13.277 | 36.227 | 68.516 | 1.00 32.02 | AAAA |
| ATOM | 1818 | CB | GLU A | | 12.399 | 36.375 | 67.272 | 1.00 30.72 | AAAA AAAA |
| ATOM | 1819 | CG | GLU A | | 11.006 | 36.896 | 67.583 | 1.00 31.02 | AAAA |
| ATOM | 1820 | CD | GLU A | | 10.175 | 37.187 | 66.350 | 1.00 31.52 | AAAA |
| ATOM | 1821 | OE1 | GLU A | | 10.644 | 37.970 | 65.497 | 1.00 31.89 | AAAA |
| ATOM | 1822 | | GLU A | | 9.047 | 36.655 | 66.241 | 1.00 31.04 | AAAA |
| ATOM | 1823 | С | GLU A | 230 | 14.628 | 35.622 | 68.180 | 1.00 30.79 | AAAA |
| ATOM | 1824 | 0 | GLU A | 230 | 14.905 | 34.465 | 68.512 | 1.00 31.05 | AAAA |
| ATOM | 1825 | N | PHE A | | 15.490 | 36.412 | 67.553 | 1.00 30.05 | AAAA |
| MOTA | 1826 | CA | PHE A | | 16.811 | 35.920 | 67.191 | 1.00 28.94 | AAAA |
| MOTA | 1827 | CB | PHE A | | 17.632 | 37.015 | 66.528 | 1.00 29.33 | AAAA |
| ATOM | 1828 | CG | PHE A | | 18.949 | 36.537 | 65.972 | 1.00 28.79 | AAAA |
| ATOM | 1829 | | PHE A | | 18.982 | 35.585 | 64.957 | 1.00 28.93 | AAAA |
| MOTA | 1830 | | PHE A | | 20.152 | 37.067 | 66.436 | 1.00 28.55 | AAAA |
| MOTA | 1831 | | PHE A | | 20.195 | 35.160 | 64.397 | 1.00 28.32 | AAAA |
| MOTA | 1832 | | PHE A | | 21.376 | 36.657 | 65.888 | 1.00 28.97 | AAAA |
| ATOM | | C | PHE A | | 21.397 | 35.695 | | 1.00 28.81 | AAAA |
| MOTA | 1834 1835 | o | PHE A | | 17.559 | 35.443 34.302 | 68.413 | 1.00 28.25 | AAAA |
| MOTA MOTA | 1836 | Ŋ | LEU A | | 17.999 17.691 | | 68.485 69.384 | 1.00 27.97 | AAAA |
| MOTA | 1837 | CA | LEU A | | 18.425 | 36.003 | 70.590 | 1.00 27.93 | AAAA |
| MOTA | 1838 | | LEU A | | 18.521 | 37.234 | 71.484 | 1.00 27.93 1.00 28.16 | AAAA |
| MOTA | 1839 | | LEU A | | 19.220 | 38.379 | 70.747 | 1.00 28.16 | AAAA AAAA |
| ATOM | 1840 | | LEU A | | 19.203 | 39.629 | 71.587 | 1.00 27.57 | AAAA |
| ATOM | 1841 | | LEU A | | 20.639 | 37.955 | 70.387 | 1.00 27.76 | AAAA |
| ATOM | 1842 | c | LEU A | | 17.815 | 34.851 | 71.340 | 1.00 27.75 | AAAA |
| ATOM | 1843 | õ | LEU A | | 18.526 | 34.061 | 71.941 | 1.00 27.92 | AAAA |
| ATCM | 1844 | | PHE A | | 16.495 | 34.758 | 71.298 | 1.00 28.81 | AAAA |
| ATOM | 1845 | CA | PHE A | | 15.786 | 33.685 | 71.972 | 1.00 30.27 | AAAA |
| ATOM | 1846 | | PHE A | 233 | 14.278 | 33.837 | 71.745 | 1.00 31.51 | AAAA |
| ATOM | 1847 | CG | PHE A | | 13.465 | 32.710 | 72.308 | 1.00 32.38 | AAAA |
| ATOM | 1848 | CD1 | PHE A | 233 | 13.257 | 32.599 | 73.677 | 1.00 33.66 | AAAA |

| | 4040 | | | | | | | | | | | |
|--------|------|-----|-----|---|-------|---|--------|----------------|---------|------|-------|--|
| MOTA | 1849 | | | | 233 | | 12.928 | 31.741 | 71.467 | 1.00 | 33.51 | AAAA |
| ATOM | 1850 | CEI | PHE | A | 233 | | 12.518 | 31.537 | 74.201 | 1.00 | 35,10 | AAAA |
| ATOM | 1851 | CE2 | PHE | A | 233 | | 12.193 | 30.677 | 71.975 | 1.00 | 34.21 | AAAA |
| ATOM | 1852 | CZ | PHE | A | 233 | | 11.986 | 30.572 | 73.344 | | 35.23 | AAAA |
| MOTA | 1853 | c | | | 233 | | 16.219 | 32.301 | 71.483 | | 30.55 | |
| | 1854 | ŏ | | | 233 | | | | | | | AAAA |
| ATOM - | | | | | | | 16.438 | 31.391 | 72.280 | | 30.65 | AAAA |
| MOTA | 1855 | N | | | 234 | | 16.317 | 32.151 | 70.165 | | 30.21 | AAAA |
| ATOM | 1856 | CA | ALA | A | 234 | | 16.698 | 30.892 | 69.549 | 1.00 | 28.97 | AAAA |
| MOTA | 1857 | CB | ALA | A | 234 | | 16.398 | 30.942 | 68.065 | | 30.40 | AAAA |
| MOTA | 1858 | С | ALA | Α | 234 | | 18.169 | 30.571 | 69.761 | | 28.27 | AAAA |
| ATOM | 1859 | ō | | | 234 | | 18.564 | 29.401 | 69.830 | | | |
| | 1860 | | | | | | | | | | 26.69 | AAAA |
| MOTA | | N | | | . 235 | | 18.978 | 31.614 | 69.855 | | 27.56 | AAAA |
| MOTA | 1861 | CA | | | 235 | • | 20.402 | 31.427 | 70.055- | 1.00 | 29.17 | AAAA |
| MOTA | 1862 | CB | LEU | A | 235 | | 21.126 | 32.767 | 69.989 | 1.00 | 29.04 | AAAA |
| ATOM | 1863 | CG | LEU | A | 235 | | 22.527 | 32.757 | 69.378 | 1.00 | 28.54 | AAAA |
| MOTA | 1864 | CD1 | LEU | A | 235 | | 23.350 | 33.837 | 70.058 | | 27.05 | - AAAA |
| ATOM | 1865 | | | | 235 | | 23.182 | 31.408 | 69.558 | | 27.21 | |
| ATOM | 1866 | c | | | 235 | | | | | | | AAAA |
| | | | | | | | 20.637 | 30.799 | 71.429 | | 30.99 | AAAA |
| MOTA | 1867 | 0 | | | 235 | | 21.159 | 29.697 | 71.547 | | 31.65 | AAAA |
| MOTA | 1868 | N | GLU | A | 236 | | 20.242 | 31.514 | 72.471 | 1.00 | 31.88 | AAAA |
| ATOM | 1869 | CA | GLU | A | 236 | | 20.409 | 31.042 | 73.838 | 1.00 | 32.99 | AAAA |
| ATOM | 1870 | CB | GLU | A | 236 | | 19.689 | 31.990 | 74.790 | 1.00 | 34.63 | AAAA |
| ATOM | 1871 | | GLU | | | | 19.980 | 33.449 | 74.531 | | 36.79 | AAAA |
| ATOM | 1872 | CD | | | 236 | | 19.044 | 34.360 | 75.294 | | 38.99 | |
| | 1873 | | GLU | | | | | | | | | AAAA |
| ATOM | • | | | | | | 17.803 | 34.303 | 75.070 | | 39.03 | AAAA |
| MOTA | 1874 | | GLU | | | | 19.559 | 35.132 | 76.126 | | 41.56 | AAAA |
| MOTA | 1875 | С | | | 236 | | 19.806 | 29.656 | 73.982 | 1.00 | 32.94 | AAAA |
| MOTA | 1876 | 0 | | | 236 | | 20.379 | 28.753 | 74.595 | 1.00 | 31.76 | AAAA |
| ATOM | 1877 | N | LYS | Α | 237 | | 18.631 | 29.503 | 73.399 | 1.00 | 32.83 | AAAA |
| ATOM | 1878 | CA | LYS | Α | 237 | | 17.906 | 28.256 | 73.471 | | 33.59 | AAAA |
| ATOM | 1879 | CB | | | 237 | | 16,504 | 28.506 | 72.942 | | 35.00 | AAAA |
| ATOM | 1880 | ĊĠ | | | 237 | | 15.516 | 27.436 | 73.213 | | 36.69 | |
| | | | | | 237 | | | | | | | AAAA |
| ATOM | 1881 | CD | | | | | 14.310 | 28.008 | 73.940 | | 38.53 | AAAA |
| MOTA | 1882 | CE | | | 237 | | 14.636 | 28.331 | 75.392 | | 39.27 | AAAA |
| ATOM | 1883 | NZ | | | 237 | | 13.398 | 28.531 | 76.204 | 1.00 | 39.42 | AAAA |
| ATOM | 1884 | С | LYS | Α | 237 | | 18.619 | 27.129 | 72.707 | 1.00 | 33.14 | AAAA |
| ATOM | 1885 | 0 | LYS | Α | 237 | | 18.850 | 26.051 | 73.260 | 1.00 | 33.29 | AAAA |
| MOTA | 1886 | N | SER | Α | 238 | | 18.985 | 27.374 | 71.452 | | 32.13 | AAAA |
| ATOM | 1887 | CA | | | 238 | | 19.671 | 26.345 | 70.685 | | 31.25 | AAAA |
| ATOM | 1888 | CB | | | 238 | | 19.740 | 26.717 | 69.194 | | 30.52 | |
| | | OG | | | | | | | | | | AAAA |
| MOTA | 1889 | | | | 238 | | 20.544 | 27.851 | 68.970 | | 29.95 | AAAA |
| MOTA | 1890 | С | | | 238 | | 21.075 | 26.064 | 71.236 | | 31.21 | AAAA |
| MOTA | 1891 | 0 | | | 238 | | 21.556 | 24.929 | 71.169 | 1.00 | 30.06 | AAAA |
| MOTA | 1892 | N | LEU | Ą | 239 | • | 21.740 | 27.07 7 | 71.782 | 1.00 | 31.71 | AAAA |
| ATOM - | 1893 | CA | LEU | A | 239 | | 23.070 | 26.842 | 72.351 | 1.00 | 33.47 | AAAA |
| MOTA | 1894 | CB | LEU | Α | 239 | | 23.698 | 28.13C | 72.900 | | 31.25 | AAAA |
| ATOM | 1895 | CG | LEU | | | | 23.988 | 29.300 | 71.977 | | 29.80 | AAAA |
| ATOM | 1896 | | LEU | | | | 24.589 | 30.414 | 72.787 | | 29.05 | AAAA |
| | | | | | | | | | | | | |
| ATOM | 1897 | | LEU | | | | 24.919 | 28.903 | 70.872 | | 29.36 | AAAA |
| MOTA | 1898 | C | LEU | | | | 22.933 | 25.839 | 73.502 | | 35.41 | AAAA |
| MOTA | 1899 | 0 | LEU | A | 239 | | 23.812 | 25.012 | 73.735 | 1.00 | 36.25 | AAAA |
| MOTA | 1900 | N | GLU | Α | 240 | | 21.816 | 25.906 | 74.213 | 1.00 | 37.34 | AAAA |
| ATOM | 1901 | CA | GLU | Α | 240 | | 21.594 | 25.005 | 75.331 | 1.00 | 39.39 | AAAA |
| ATOM | 1902 | CB | GLU | | | | 20.281 | 25.361 | 76.017 | | 41.90 | AAAA |
| ATOM | 1903 | CG | GLU | | | | 20.040 | 24.610 | 77.308 | | 45.52 | AAAA |
| | 1904 | CD | GLU | | | | 19.665 | 25.552 | 78.432 | | | |
| MOTA | | | | | | | | | | | 47.80 | AAAA |
| MOTA | 1905 | | GLU | | | | 18.670 | 26.295 | 78.274 | | 49.70 | AAAA |
| MOTA | 1906 | | GLU | | | | 20.364 | 25.559 | 79.469 | | 48.04 | AAAA. |
| MOTA | 1907 | С | GLU | Α | 240 | | 21.583 | 23.555 | 74.875 | 1.00 | 38.80 | AAAA |
| MOTA | 1908 | o | GLU | А | 240 | | 22.224 | 22.700 | 75.478 | 1.00 | 37.85 | AAAA |
| ATOM | 1909 | N | ILE | | | | 20.847 | 23.293 | 73.804 | | 39.66 | AAAA |
| ATOM | 1910 | CA | ILE | | | | 20.751 | 21.955 | 73.223 | | 40.81 | AAAA |
| | 1911 | | ILE | | | | 19.912 | 21.994 | 71.917 | | | |
| ATOM | | CB | | | | | | | | | 41.10 | AAAA |
| MOTA | 1912 | | ILE | | | | 19.850 | 20.621 | 71.287 | | 40.88 | AAAA |
| ATOM | 1913 | | ILE | | | | 18.502 | 22.514 | 72.220 | | 41.45 | AAAA |
| MOTA | 1914 | CD1 | ILE | A | 241 | | 17.641 | 22.745 | 70.992 | 1.00 | 41.14 | AAAA |
| | | | | | | | | | | | | the state of the s |

| | | | | • | | | | | | * |
|--------------|----------------|----------|---------|-----|------------------|------------------|------------------|--------|-------|--------------|
| ATOM | 1915 | С | ILE A 2 | 241 | 22.159 | 21.424 | 72.893 | 1.00 4 | 1.66 | AAAA |
| ATOM | 1916 | 0 | ILE A 2 | 241 | 22.445 | 20.229 | 73.045 | 1.00 4 | 2.10 | AAAA |
| ATOM | 1917 | N | VAL A | 242 | 23.026 | 22.324 | 72.432 | 1.00 4 | | AAAA |
| MOTA | 1918 | CA | VAL A 2 | 242 | 24.394 | 21.977 | 72.076 | 1.00 4 | | AAAA |
| MOTA | 1919 | CB | VAL A | 242 | 25.089 | 23.146 | 71.351 | 1.00 4 | | AAAA |
| MOTA | 1920 | | VAL A | | 26.556 | 22.850 | 71.171 | 1.00 3 | | AAAA |
| MOTA | 1921 | CG2 | VAL A 2 | | 24.438 | 23.384 | 70.004 | 1.00 3 | | AAAA |
| MOTA | 1922 | С | VAL A | 242 | 25.228 | 21.604 | 73.298 | 1.00 4 | | AAAA |
| ATOM | 1923 | 0 | VAL A | 242 | 25.882 | 20.562 | 73.316 | 1.00 4 | | AAAA |
| ATOM | 1924 | N | LYS A | | 25.198 | 22.456 | 74.318 | 1.00 4 | | AAAA |
| ATOM | 1925 | CA | LYS A | | 25.972 | 22.215 | 75.523 | 1.00 4 | | AAAA |
| MOTA | 1926 | CB | LYS A | | 25.797 | 23.363 | 76.522 | 1.00 4 | | AAAA |
| MOTA | 1927 | CG | LYS A | | 26.820 | 23.312 | 77.664 | 1.00 4 | | AAAA · |
| ATOM | 1928 | CD | LYS A | | 26.479 | 24.248 | 78.823 | 1.00 4 | | AAAA |
| MOTA | 1929 | CE | LYS A | | 26.355 | 25.691 | 78.380 79.505 | 1.00 4 | | AAAA AAAA |
| MOTA | 1930 | NZ | LYS A | | 25.926 | 26.576 | 76.209 | 1.00 | | AAAA |
| MOTA | 1931 | C | LYS A | | 25.639 | 20.891 | 76.711 | 1.00 | | AAAA |
| MOTA | 1932 | 0 | LYS A | | 26.537 24.362 | 20.216 20.517 | 76.237 | 1.00 | | AAAA |
| MOTA | 1933 | N | GLU A | | 23.957 | 19.262 | 76.877 | 1.00 | | AAAA |
| MOTA | 1934 | CA | GLU A | | 22.432 | 19.208 | 77.103 | 1.00 | | AAAA |
| MOTA | 1935 | CB | GLU A | | 21.818 | 20.405 | 77.829 | 1.00 | | AAAA |
| MOTA | 1936 | CG | GLU A | | 20.359 | 20.174 | 78.230 | 1.00 | | AAAA |
| ATOM | 1937 1938 | CD | GLU A | | 19.666 | 21.158 | 78.595 | 1.00 | | AAAA |
| ATOM | 1939 | OE2 | GLU A | | 19.912 | 19.006 | 78.200 | 1.00 | | AAAA |
| MOTA MOTA | 1940 | C | GLU A | | 24.338 | 18.046 | 76.033 | 1.00 | 51.06 | AAAA |
| ATOM | 1941 | ō | GLU A | | 24.206 | 16.905 | 76.477 | 1.00 | 51.68 | AAAA |
| MOTA | 1942 | N | VAL A | | 24.810 | 18.292 | 74.820 | 1.00 | 51.12 | AAAA |
| MOTA | 1943 | CA | VAL A | 245 | 25.149 | 17.212 | 73.904 | 1.00 | 50.08 | AAAA |
| ATOM | 1944 | CB | VAL A | 245 | 24.217 | 17.263 | 72.677 | 1.00 | | AAAA |
| ATOM | 1945 | CG1 | VAL A | 245 | 24.615 | 16.217 | 71.651 | 1.00 | | AAAA |
| ATOM | 1946 | CG2 | VAL A | 245 | 22.794 | 17.049 | 73.118 | 1.00 | | AAAA |
| ATOM | 1947 | С | VAL A | 245 | 26.578 | 17.254 | 73.397 | 1.00 | | AAAA |
| ATOM | 1948 | 0 | VAL A | | 27.101 | 16.250 | 72.917 | 1.00 | | AAAA |
| ATOM | 1949 | N | PHE A | | 27.220 | 18.408 | 73.522 | 1.00 | | AAAA AAAA |
| ATOM | 1950 | CA | PHE A | | 28.556 | 18.552 | 72.982 71.607 | 1.00 | | AAAA |
| MOTA | 1951 | CB | PHE A | | 28.420 | 19.212 18.932 | 70.671 | 1.00 | | AAAA |
| ATOM | 1952 | CG | PHE A | | 29.553 29.841 | 17.629 | 70.280 | 1.00 | | AAAA |
| MOTA | 1953 | | PHE A | | 30.291 | 19.972 | 70.124 | 1.00 | | AAAA |
| ATOM | . 1954 1955 | | PHE A | | 30.840 | 17.370 | 69.356 | 1.00 | | AAAA |
| MOTA MOTA | 1956 | | PHE A | | 31.292 | 19.721 | 69.197 | 1.00 | 43.47 | AAAA |
| ATOM | 1957 | CZ | PHE A | | 31.566 | 18.422 | 68.811 | 1.00 | 44.05 | AAAA |
| MOTA | 1958 | c | PHE A | | 29.481 | 19.383 | 73.860 | 1.00 | 48.60 | AAAA |
| ATOM | 1959 | ō | PHE A | | 29.132 | 20.501 | 74.239 | 1.00 | 49.59 | AAAA |
| ATOM | 1960 | N | GLU A | 247 | 30.647 | 18.834 | 74.198 | | 48.69 | AAAA |
| ATOM. | 1961 | CA | GLU A | 247 | 31.644 | 19.578 | 74.977 | | 49.45 | AAAA |
| ATOM | 1962 | CB | GLU A | | 32.174 | 18.768 | 76.178 | | 51.91 | AAAA |
| MOTA | 1963 | CG | GLU A | | 31.257 | 18.659 | 77.398 | | 54.39 | AAAA |
| MOTA | 1964 | CD | GLU A | | 29.986 | 17.845 | 77.146 | | 57.34 | AAAA AAAA |
| ATOM | 1965 | OE1 | GLU A | 247 | 29.100 | 18.315 | 76.393 77.702 | 1.00 | 58.48 | AAAA |
| MOTA | 1966 | | GLU A | | 29.877 | 16.725 | 74.024 | 1.00 | | AAAA |
| MOTA | 1967 | C | GLU A | | 32.807 | 19.903 | 73.872 | | 46.65 | AAAA |
| MOTA | 1968 | 0 | GLU A | | 33.742 | 19.119 | 73.371 | | 46.25 | AAAA |
| MOTA | 1969 | N | PRO A | | 32.748 | 21.070 | 73.543 | | 46.49 | AAAA |
| ATOM | 1970 | CD | PRO A | | 31.651 | 22.033 21.614 | 72.411 | | 45.44 | AAAA |
| MOTA | 1971 | CA | PRO A | | 33.710 33.063 | 22.948 | 72.017 | | 45.57 | AAAA |
| MOTA | 1972 | CB CG | PRO A | | 31.604 | 22.661 | 72.178 | | 46.28 | AAAA |
| ATOM | 1973 | C | PRO A | | 35.155 | 21.814 | 72.880 | | 44.29 | AAAA |
| ATOM | 1974 | 0 | PRO A | | 35.401 | 22.370 | 73.947 | | 44.57 | AAAA |
| ATOM | 1975 1976 | Ŋ | GLU A | | 36.100 | 21.364 | 72.059 | | 42.21 | AAAA |
| ATOM | 1977 | CA | GLU A | | 37.522 | 21.526 | 72.340 | | 39.87 | AAAA |
| ATOM | 1978 | CB | GLU A | | 38.344 | 20.460 | 71.625 | | 39.58 | AAAA |
| MOTA MOTA | 1979 | ÇG | GLU A | | 37.960 | 19.030 | 71.957 | | 41.32 | AAAA |
| ATOM | 1980 | CD | GLU A | | 38.825 | 18.007 | 71.241 | 1.00 | 40.96 | AAAA |
| VION | 2200 | ٠ | | | • | | - | | | • |

| MOTA | 1981 | OE1 | GLU | A 249 | 38.87 1 | 18.017 | 69.996 | 1.00 41.55 | AAAA |
|------|------|------|-------|--------|----------------|--------|--------|------------|------|
| MOTA | 1982 | OE2 | GLU . | A 249 | 39.462 | 17.187 | 71.926 | 1.00 42.49 | AAAA |
| ATOM | 1983 | С | _ | A 249 | 37.840 | 22.873 | 71.718 | 1.00 38.81 | AAAA |
| | 1984 | ō | | A 249 | 38.715 | 23.617 | 72.181 | 1.00 38.27 | |
| MOTA | | | | | | | | | AAAA |
| ATOM | 1985 | Ŋ | | A 250 | 37.109 | 23.160 | 70.644 | 1.00 36.60 | AAAA |
| ATOM | 1986 | CA | | A 250 | 37.242 | 24.402 | 69.890 | 1.00 34.20 | AAAA |
| ATOM | 1987 | CB | VAL . | A 250 | 38.379 | 24.321 | 68.862 | 1.00 33.73 | AAAA |
| MOTA | 1988 | CG1 | VAL . | A 250 | 38.085 | 23.209 | 67.864 | 1.00 33.26 | AAAA |
| ATOM | 1989 | CG2 | VAL. | A. 250 | 38.546 | 25.678 | 68.153 | 1.00 33.75 | AAAA |
| ATOM | 1990 | c | | A 250 | 35.945 | 24.617 | 69.130 | 1.00 31.98 | AAAA |
| | 1991 | ō | | A 250 | 35.205 | 23.658 | 68.904 | 1.00 32.36 | AAAA |
| MOTA | | | | | | | | | |
| MOTA | 1992 | N | | A 251 | 35.657 | 25.863 | 68.760 | 1.00 28.65 | AAAA |
| MOTA | 1993 | CA | | A 251 | 34.449 | 26.150 | 67.991 | 1.00 26.49 | AAAA |
| MOTA | 1994 | CB | | A 251 | 33.241 | 26.442 | 68.906 | 1.00 24.32 | AAAA |
| MOTA | 1995 | CG | TYR . | A 251 | 33.193 | 27.853 | 69.465 | 1.00 22.96 | AAAA |
| MOTA | 1996 | CD1 | TYR . | A 251 | 32.771 | 28.931 | 68.668 | 1.00 22.21 | AAAA |
| ATOM | 1997 | CE1 | TYR . | A 251 | 32.791 | 30.234 | 69.151 | 1.00 21.29 | AAAA |
| MOTA | 1998 | | | A 251 | 33.628 | 28.124 | 70.771 | 1.00 21.47 | AAAA |
| | | CE2 | | A 251 | 33.651 | 29.425 | 71.265 | 1.00 20.80 | AAAA |
| MOTA | 1999 | | | | | | | | |
| ATOM | 2000 | CZ | | A 251 | 33.237 | 30.475 | 70.449 | 1.00 20.77 | AAAA |
| MOTA | 2001 | OH | | A 251 | 33.309 | 31.768 | 70.913 | 1.00 21.41 | AAAA |
| MOTA | 2002 | С | | A 251 | 34.691 | 27.345 | 67.092 | 1.00 24.59 | AAAA |
| ATOM | 2003 | 0 | TYR : | A 251 | 35.504 | 28.216 | 67.410 | 1.00 25.87 | AAAA |
| ATOM | 2004 | N | LEU : | A 252 | 33.984 | 27.374 | 65.970 | 1.00 22.49 | AAAA |
| MOTA | 2005 | CA | LEU . | A 252 | 34.082 | 28.482 | 65.045 | 1.00 20.96 | AAAA |
| ATOM | 2006 | CB | | A 252 | 34.523 | 28.018 | 63.657 | 1.00 21.31 | AAAA |
| MOTA | 2007 | CG | | A 252 | 35.940 | 27.472 | 63.556 | 1.00 21.03 | AAAA |
| | 2008 | | LEU | | 35.947 | 26.028 | 63.977 | 1.00 22.16 | AAAA |
| MOTA | | | | | | | | 1.00 22.13 | |
| MOTA | 2009 | | LEU A | | 36.440 | 27.594 | 62.143 | | |
| MOTA | 2010 | C | | A 252 | 32.731 | 29.159 | 64.959 | 1.00 19.60 | AAAA |
| MOTA | 2011 | 0 | | A 252 | 31.689 | 28.523 | | 1.00 19.95 | AAAA |
| MOTA | 2012 | N | LEU A | A 253 | 32.748 | 30.461 | 64.756 | 1.00 17.95 | AAAA |
| MOTA | 2013 | CA | LEU 2 | A 253 | 31.521 | 31.222 | 64.675 | 1.00 17.33 | AAAA |
| MOTA | 2014 | CB | LEU A | A 253 | 31.441 | 32.142 | 65.900 | 1.00 16.31 | AAAA |
| MOTA | 2015 | CG | LEU A | A 253 | 30.266 | 33.070 | 66.153 | 1.00 15.81 | AAAA |
| ATOM | 2016 | | LEU Z | | 28.990 | 32.267 | 66.377 | 1.00 14.74 | AAAA |
| ATOM | 2017 | | LEU A | | 30.602 | 33.925 | 67.368 | 1.00 15.83 | AAAA |
| | | C | | A 253 | 31.564 | 32.035 | 63.386 | 1.00 16.60 | AAAA |
| MOTA | 2018 | | | | | | | | |
| MOTA | 2019 | 0 | | A 253 | 32.548 | 32.722 | 63.132 | 1.00 16.40 | AAAA |
| ATOM | 2020 | N | | A 254 | 30.526 | 31.936 | 62.557 | 1.00 15.88 | AAAA |
| MOTA | 2021 | CA | | A 254 | 30.507 | 32.716 | 61.328 | 1.00 16.27 | AAAA |
| ATOM | 2022 | CB | GLN A | A 254 | 30.045 | 31.881 | 60.121 | 1.00 15.88 | AAAA |
| MOTA | 2023 | CG | GLN A | A 254 | 28.587 | 32.048 | 59.734 | 1.00 18.52 | AAAA |
| MOTA | 2024 | CD | GLN A | A 254 | 28.380 | 32.935 | 58.519 | 1.00 17.54 | AAAA |
| ATOM | 2025 | OE1 | GLN A | A 254 | 28.714 | 32.572 | 57.391 | 1.00 15.89 | AAAA |
| ATOM | 2026 | | GLN A | | 27.828 | 34.103 | 58.750 | 1 00 18.49 | AAAA |
| ATOM | 2027 | c | GLN A | | 29.527 | 33.825 | 61.650 | 1 00 16.91 | AAAA |
| | | õ | GLN 2 | | 28.450 | 33.571 | 62.198 | | AAAA |
| ATOM | 2028 | | | | | | 61.319 | 1.00 16.68 | AAAA |
| ATOM | 2029 | N | LEU A | | 29.911 | 35.053 | | | |
| MOTA | 2030 | CA | LEU A | | 29.102 | 36.215 | 61.619 | 1.00 16.42 | AAAA |
| MOTA | 2031 | CB | LEU A | | | 37.080 | | | AAAA |
| MOTA | 2032 | · CG | LEU A | | 30.269 | 36.301 | 63.860 | 1.00 13.90 | AAAA |
| MOTA | 2033 | CD1 | LEU A | 1 255 | 31.494 | 36.924 | 64.515 | 1.00 12.24 | AAAA |
| ATOM | 2034 | CD2 | LEU A | 255 | 29.083 | 36.202 | 64.774 | 1.00 12.80 | AAAA |
| ATOM | 2035 | C | LEU A | | 28.699 | 37.048 | 60.404 | 1.00 18.32 | AAAA |
| | 2036 | ō | LEU A | | 29.170 | 38.177 | 60.216 | 1.00 17.59 | AAAA |
| MOTA | | | GLY A | | 27.813 | 36.482 | 59.588 | 1.00 19.75 | AAAA |
| MOTA | 2037 | N | | | | | | | |
| MOTA | 2038 | CA | GLY A | | 27.322 | 37.188 | 58.422 | 1.00 20.77 | AAAA |
| ATOM | 2039 | C | GLY A | | 26.422 | 38.302 | 58.927 | 1.00 21.73 | AAAA |
| MOTA | 2040 | 0 | GLY A | 256 | 25 .642 | 3ა.096 | 59.857 | 1.00 21.38 | AAAA |
| ATOM | 2041 | N | THR A | 257 | 26.528 | 39.485 | 58.325 | 1.00 22.82 | AAAA |
| ATOM | 2042 | CA | THR A | | 25.721 | 40.622 | 58.746 | 1.00 23.85 | AAAA |
| MOTA | 2043 | СВ | THR A | | 26.460 | 41.968 | 58.549 | 1.00 23.99 | AAAA |
| | 2044 | 061 | THR A | | 26.729 | 42.169 | 57.153 | 1.00 25.54 | AAAA |
| ATOM | | | THR A | | 27.780 | 41.985 | 59.329 | 1.00 24.07 | AAAA |
| MOTA | 2045 | | | | 24.438 | | | 1.00 24.97 | AAAA |
| MOTA | 2046 | C· | THR A | 441 | 44.430 | 40.691 | 57.948 | 2.00 44.3/ | Anna |

247/263 Figure 19-32

| MOTA | 2047 | 0 | THR | A | 257 | 23.692 | 41.672 | 58.048 | 1.00 | 25.84 | | AAAA |
|--------|-------|-----|-----|---|-------|--------|--------|--------------------|------|-------|---|------|
| ATOM | 2048 | N | | | 258 | 24.152 | 39.665 | 57.154 | | 25.18 | | AAAA |
| | 2049 | CA | | | 258 | 22.935 | 39.753 | 56.379 | | 26.18 | | |
| ATOM | | | | | | | | | | | | AAAA |
| ATOM | 2050 | CB | | | 258 | 22.950 | 38.830 | 55.149 | | 25.52 | | AAAA |
| MOTA | 2051 | CG | | | 258 | 23.211 | 37.392 | 55.494 | 1.00 | 26.33 | | AAAA |
| ATOM | 2052 | С | ASP | A | 258 | 21.649 | 39:574 | 57.178 | 1.00 | 26.74 | | AAAA |
| ATOM | 2053. | 0 | ASP | A | 258 | 20.571 | 39.823 | 56.643 | 1.00 | 26.57 | | AAAA |
| ATOM | 2054 | | ASP | | | 23.014 | 37.029 | 56.675 | | 26.85 | | AAAA |
| | 2055 | | ASP | | • | | | | | | | |
| ATOM | | | | | | 23.585 | 36:623 | 54.572 | | 24.06 | | AAAA |
| ATOM | 2056 | N | | | 259 | 21.727 | 39.114 | 58.449 | | 26.95 | | AAAA |
| MOTA | 2057 | CD | PRO | Α | 259 . | 22.834 | 38.589 | 59.271 | 1.00 | 27.34 | | AAAA |
| ATOM | 2058 | CA | PRO | Α | 259 | 20.467 | 38.976 | 59.190 | 1.00 | 27.05 | | AAAA |
| ATOM | 2059 | CB | PRO | Α | 259 | 20.886 | 38.186 | 60.425 | 1.00 | 26.38 | | AAAA |
| ATOM | 2060 | CG | | | 259 | 22.247 | 38.718 | 60.669 | | 27.84 | | AAAA |
| ATOM | 2061 | c | | | 259 | 19.914 | 40.365 | 59.543 | | 27.32 | | AAAA |
| | | | | | | | | | | | | |
| ATOM | 2062 | 0 | | | 259 | 18.739 | 40.510 | 59.871- | | 27.29 | | AAAA |
| ATOM | 2063 | N | | | 260 | 20.771 | 41,383 | 59.452 | | 26.97 | | AAAA |
| ATOM | 2064 | CA | LEU | Α | 260 | 20.389 | 42.763 | 59.752 | 1.00 | 26.74 | | AAAA |
| ATOM | 2065 | CB | LEU | A | 260 | 21.621 | 43.680 | 59.680 | 1.00 | 27.21 | | AAAA |
| MOTA | 2066 | CG | LEU | Α | 260 | 22.732 | 43.465 | 60.709 | 1.00 | 27.01 | | AAAA |
| ATOM | 2067 | | LEU | | | 23.889 | 44.380 | 60.408 | | 25.51 | | AAAA |
| | 2068 | | LEU | | | 22.189 | 43.718 | 62.112 | | 27.39 | | |
| ATOM | | | | | | | | | | | | AAAA |
| ATOM | 2069 | Ċ | | | 260 | 19.295 | 43.351 | 58.865 | | 26.47 | | AAAA |
| ATOM | 2070 | 0 | | | 260 | 19.278 | 43.137 | 57.649 | | 26.72 | | AAAA |
| ATOM . | 2071 | И | LEU | A | 261 | 18.413 | 44.126 | 59.494 | 1.00 | 26.32 | | AAAA |
| ATOM | 2072 | CA | LEU | A | 261 | 17.283 | 44.808 | 58.846 | 1.00 | 27.20 | | AAAA |
| ATOM | 2073 | CB | LEU | Α | 261 | 16.732 | 45.885 | 59.780 | 1.00 | 28.71 | | AAAA |
| ATOM | 2074 | CG | LEU | Α | 261 | 15.644 | 46.789 | 59.190 | 1.00 | 29.24 | | AAAA |
| ATOM | 2075 | | LEU | | | 14.433 | 45.954 | 58.883 | | 29.44 | | AAAA |
| ATOM - | 2076 | | LEU | | | 15.284 | 47.906 | 60.162 | | 29.72 | | AAAA |
| | | | | | | | | | | 27.90 | | |
| MOTA | 2077 | C | LEU | | | 17.506 | 45.454 | 57.473 | | - | | AAAA |
| ATOM | 2078 | 0 | LEU | | | 16.675 | 45.294 | 56.577 | | 28.21 | | AAAA |
| ATOM | 2079 | И | GLU | A | 262 | 18.597 | 46.202 | 57.310 | | 27.61 | • | AAAA |
| ATOM | 2080 | CA | GLU | А | 262 · | 18.887 | 46.877 | 56.043 | 1.00 | 26.92 | | AAAA |
| ATOM | 2081 | CB | GLU | Α | 262. | 19.949 | 47.955 | 56.241 | 1.00 | 25.85 | | AAAA |
| ATOM | 2082 | CG | GLU | Α | 262 | 19.549 | 49.119 | 57.117 | 1.00 | 25.36 | | AAAA |
| ATOM | 2083 | CD | GLU | | | 19.552 | 48.787 | 58.580 | | 25.78 | | AAAA |
| ATOM | 2084 | | GLU | | | 19.859 | 47.631 | 58.938 | | 24.64 | | AAAA |
| | | | | | | | | | | 25.82 | | |
| ATOM | 2085 | OE2 | GLU | | | 19.255 | 49.694 | 59.381 | | | | AAAA |
| MOTA | 2086 | С | GLU | | | 19.346 | 45.995 | 54.882 | | 28.79 | | AAAA |
| ATOM | 2087 | 0 | GLU | | | 19.354 | 46.439 | 53.724 | | 28.70 | | AAAA |
| ATOM | 2088 | N. | ASP | | | 19.743 | 44.758 | 55.17 9 | 1.00 | 29.57 | | AAAA |
| ATOM | 2089 | CA | ASP | A | 263 | 20.230 | 43.853 | 54.145 | 1.00 | 28.99 | | AAAA |
| ATOM | 2090 | CB | ASP | Α | 263 | 21.160 | 42.802 | 54.760 | 1.00 | 27.89 | | AAAA |
| ATOM | 2091 | CG | ASP | | | 21.986 | 42.062 | 53.714 | 1.00 | 29.02 | | AAAA |
| ATOM | 2092 | | ASP | | | 23.194 | 41.863 | 53.957 | | 28.06 | | AAAA |
| | 2093 | | ASP | | | 21.438 | 41.663 | 52.660 | | 28.80 | | AAAA |
| ATOM | | | | | | | | | | | | |
| MOTA | 2094 | C | ASP | | | 19.066 | 43.197 | 53.431 | | 29.73 | • | AAAA |
| MOTA | 2095 | 0 | ASP | | | 18.258 | 42.510 | 54.043 | | 29.15 | | AAAA |
| MOTA | 2096 | N | TYR | Α | 264 | 19.002 | 43.416 | 52.122 | | 31.25 | | AAAA |
| ATOM | 2097 | CA | TYR | A | 264 | 17.925 | 42.888 | 51.306 | 1.00 | 32.43 | | AAAA |
| ATOM | 2098 | CB | TYR | Α | 264 | 17.913 | 43.558 | 49.938 | 1.00 | 34.53 | | AAAA |
| MOTA | 2099 | CG | TYR | | | 17.627 | 45.038 | 49.997 | | 38.21 | | AAAA |
| | 2100 | | TYR | | | 18.664 | | 49.983 | | 39.87 | | AAAA |
| ATOM | | | | | | | | | | | | |
| ATOM | 2101 | CEL | TYR | | | 18.409 | 47.335 | 50.068 | | 41.74 | | AAAA |
| ATOM | 2102 | | TYR | | | 16.316 | 45.511 | 50.103 | | 40.10 | | AAAA |
| MOTA | 2103 | CE2 | TYR | | | 16.044 | 46.877 | 50.191 | | 41.50 | | AAAA |
| MOTA | 2104 | CZ | TYR | A | 264 | 17.095 | 47.786 | 50.170 | 1.00 | 42.75 | | AAAA |
| MOTA | 2105 | OH | TYR | | | 16.838 | 49.147 | 50.231 | 1.00 | 44.65 | | AAAA |
| ATOM | 2106 | c | TYR | | | 17.897 | 41.385 | 51.135 | | 32.50 | | AAAA |
| | 2107 | õ | TYR | | | 16.819 | 40.816 | 50.968 | | 32.49 | | AAAA |
| ATOM | | | | | | | | | | 32.64 | | |
| ATOM | 2108 | И | LEU | | | 19.064 | 40.740 | 51.171 | | | | AAAA |
| ATOM | 2109 | CA | LEU | | | 19.122 | 39.281 | 51.036 | | 31.92 | | AAAA |
| MOTA | 2110 | CB | LEU | | | 20.525 | 38.823 | 50.617 | | 32.75 | | AAAA |
| ATOM | 2111 | CG | LEU | | | 20.808 | 39.010 | 49.127 | | 32.95 | | AAAA |
| ATOM | 2112 | CD1 | LEU | A | 265 | 22.213 | 38.588 | 48.771 | 1.00 | 31.59 | | AAAA |
| | - | | | | | | | - | | | | |

Figure 19-33

| MOTA | 2113 | CD2 | LEU A | 265 | 19.803 | 38.166 | 48.361 | 1.00 34.62 | AAAA |
|--------|------|-----|-------|------|--------------|---------|--------|------------|--------|
| | 2114 | С | LEU A | 265 | 18.693 | 38.540 | 52.296 | 1.00 30.33 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 2115 | 0 | LEU A | 265 | 19.024 | 37.375 | 52.484 | 1.00 30.30 | AAAA |
| MOTA | 2116 | N | SER A | 266 | 17.945 | 39.230 | 53.147 | 1.00 29.23 | AAAA |
| | 2117 | CA | SER A | | 17.434 | 38.649 | 54.371 | 1.00 29.72 | AAAA |
| MOTA | | | | | | | | | |
| - MOTA | 2118 | CB | SER A | 266 | 18.398 | 38.894 | 55.519 | 1.00 32.09 | AAAA |
| MOTA | 2119 | OG | SER A | 266 | 17.728 | 38.810 | 56.771 | 1.00 33.43 | AAAA |
| | 2120 | C | SER A | | 16.115 | 39.290 | 54.698 | 1.00 28.71 | ÀAAA |
| ATOM | | | | | | | | | |
| MOTA | 2121 | 0 | SER A | 266 | 15.924 | 40.473 | 54.444 | 1.00 29.67 | AAAA |
| ATOM | 2122 | N | LYS A | 267 | 15.209 | 38.517 | 55.276 | 1.00 27.82 | AAAA |
| | | | | | 13.908 | | 55.654 | 1.00 27.56 | AAAA |
| MOTA | 2123 | CA | LYS A | | | 39.045 | | | |
| MOTA | 2124 | CB | LYS A | .267 | 12.821 | 38.076 | 55.222 | 1.00 28.75 | AAAA |
| MOTA | 2125 | CG | LYS A | 267 | 12.733 | 37.922 | 53.718 | 1.00 29.67 | AAAA |
| | | | LYS A | | 12.343 | 39.223 | 53.053 | 1.00 30.13 | AAAA |
| MOTA | 2126 | CD | | | | | | | |
| ATOM | 2127 | CE | LYS A | 267 | 12.303 | 39.036 | 51.546 | 1.00 31.86 | AAAA |
| ATOM | 2128 | NZ | LYS A | 267 | 11.796 | 40.252 | 50.843 | 1.00 33.92 | -AAAA |
| | | | LYS A | | 13.800 | 39.327 | 57.152 | 1.00 27.18 | AAAA |
| atom | 2129 | C | | | | | | | |
| MOTA | 2130 | 0 | LYS A | 267 | 12.707 | 39.591 | 57.665 | 1.00 27.18 | AAAA |
| ATOM | 2131 | N | PHE A | 268 | 14.944 | 39.267 | 57.836 | 1.00 26.12 | AAAA |
| | 2132 | CA | PHE A | | 15.048 | 39.532 | 59.271 | 1.00 25.72 | AAAA |
| MOTA | | | | | | | | | |
| MOTA | 2133 | CB | PHE A | 268 | 16.272 | 38.830 | 59.856 | 1.00 24.94 | AAAA |
| ATOM. | 2134 | CG | PHE A | 268 | 16.167 | 37.334 | 59.896 | 1.00 25.07 | AAAA |
| ATOM | 2135 | CDI | PHE A | 268 | 17.271 | 36.565 | 60.267 | 1.00.24.56 | AAAA |
| | | | | | | | | | |
| ATOM | 2136 | CD2 | PHE A | | 14.955 | 36.687 | 59.629 | 1.00 23.76 | AAAA |
| MOTA | 2137 | CE1 | PHE A | 268 | 17.174 | 35.169 | 60.384 | 1.00 23.71 | AAAA |
| ATOM | 2138 | CE2 | PHE A | 268 | 14.850 | 35.303 | 59.739 | 1.00 23.86 | AAAA |
| | | | | | | | | | |
| MOTA | 2139 | CZ | PHE A | | 15.966 | 34.542 | 60.121 | 1.00 23.68 | AAAA |
| ATOM | 2140 | С | PHE A | 268 | 15.190 | 41.030 | 59.513 | 1.00 25.77 | AAAA |
| MOTA | 2141 | 0 | PHE A | 268 | 15.811 | 41.734 | 58.726 | 1.00 25.81 | AAAA |
| | | Ŋ | ASN A | | 14.606 | | 60.595 | 1.00 26.02 | AAAA |
| MOTA | 2142 | | | | | | | | |
| MOTA | 2143 | CA | ASN A | 269 | 14.718 | 42.943 | 60.890 | 1.00 26.58 | AAAA |
| MOTA | 2144 | CB | ASN A | 269 | 13.330 | 43.584 | 61.058 | 1.00 25.47 | AAAA |
| ATOM | 2145 | CG | ASN A | | 12.379 | 43.252. | 59.906 | 1.00 25.37 | AAAA |
| | | | | | | | | | |
| MOTA | 2146 | ODI | ASN A | 269 | 12.761 | 43.260 | 58.734 | 1.00 23.82 | AAAA |
| MOTA | 2147 | ND2 | ASN A | 269 | 11.123 | 42.985 | 60.245 | 1.00 24.03 | AAAA |
| ATOM | 2148 | С | ASN A | 269 | 15.540 | 43.112 | 62.169 | 1.00 26.82 | AAAA |
| | | | | | | | | 1.00 27.98 | |
| MOTA | 2149 | 0 | ASN A | | 15.089 | 43.715 | 63.150 | | AAAA |
| ATOM | 2150 | N | LEU A | 270 | 16.744 | 42.559 | 62.149 | 1.00 26.07 | AAAA |
| MOTA | 2151 | CA | LEU A | 270 | 17.639 | 42.642 | 63.289 | 1.00 25.97 | AAAA |
| | 2152 | CB | LEU A | | 18.634 | 41.479 | 63.265 | 1.00 23.76 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2153 | CG | LEU A | | 18.048 | 40.070 | 63.225 | 1.00 23.36 | AAAA |
| ATOM | 2154 | CD1 | LEU A | 270 | 19.115 | 39.090 | 63.710 | 1.00 21.90 | AAAA |
| ATOM | 2155 | CD2 | LEU A | 270 | 16.824 | 39.971 | 64.122 | 1.00 22.05 | AAAA |
| | | | | | | | 63.360 | 1.00 27.13 | AAAA |
| MOTA | 2156 | C | LEU A | | 18.420 | 43.961 | | | |
| ATOM | 2157 | 0 | LEU A | 270 | 18.475 | 44.750 | 62.399 | 1.00 25.99 | AAAA |
| ATOM | 2158 | N | SER A | 271 | 19.038 | 44.176 | 64.517 | 1.00 27.97 | : AAAA |
| | 2159 | CA | SER A | | 19.832 | 45.370 | 64.767 | 1.00 27.95 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2160 | CB | SER A | | 19.235 | 46.137 | 65.943 | 1.00 27.32 | AAAA |
| ATOM | 2161 | OG | SER A | 271 | 19.184 | 45.297 | 67.089 | 1.00 27.90 | AAAA |
| ATOM | 2162 | С | SER A | 271 | 21.276 | 44.987 | 65.084 | 1.00 28.15 | AAAA |
| | | ō | SER A | | 21.574 | 43.832 | 65.401 | 1.00 26.99 | AAAA |
| MOTA | 2163 | | | | | | | | |
| MOTA | 2164 | N | ASN A | 272 | 22.156 | 45.980 | 64.979 | 1.00 28.96 | AAAA |
| MOTA | 2165 | CA | ASN A | 272 | 23.590 | 45.861 | 65.266 | 1.00 29.54 | AAAA |
| | 2166 | CB | ASN A | | 24.247 | 47.243 | 65.223 | 1.00 30.96 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 2167 | CG | ASN A | 272 | 24.647 | 47.640 | 63.850 | 1.00 31.20 | AAAA |
| ATOM | 2168 | OD1 | ASN A | 272 | 24.960 | 48.794 | 63.594 | 1.00 31.73 | AAAA |
| | 2169 | | ASN A | | 24.670 | 46.674 | 62.948 | 1.00 31.93 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2170 | С | ASN A | | 23.821 | 45.309 | 66.645 | 1.00.29.63 | AAAA |
| ATOM | 2171 | 0 | ASN A | 272 | 24.574 | 44.361 | 66.843 | 1.00 29.85 | AAAA |
| | 2172 | N | VAL A | | 23.180 | 45.959 | 67.600 | 1.00 29.77 | AAAA |
| MOTA | | | | | | | | 1.00 30.89 | AAAA |
| MOTA | 2173 | CA | VAL A | | 23.290 | 45.602 | 68.994 | | |
| ATOM | 2174 | CB | VAL A | 273 | 22.436 | 46.576 | 69.816 | 1.00 31.61 | AAAA |
| | 2175 | | VAL A | 273 | 22.716 | 46.403 | 71.293 | 1.00 33.17 | AAAA |
| MOTA | | | | | | | 69.372 | 1.00 31.82 | AAAA |
| MOTA | 2176 | | VAL A | | 22.740 | 47.998 | | | |
| MOTA | 2177 | C | VAL A | | 22.883 | 44.144 | 69.266 | 1.00 30.74 | AAAA |
| MOTA | 2178 | 0 | VAL A | 273 | 23.550 | 43.431 | 70.022 | 1.00 31.23 | AAAA . |
| WION | | - | | | - | | • | _ | _ |

SUBSTITUTE SHEET (RULE 26)

| MOTA | 2179 | N | ALA A | 274 | 21.785 | 43.706 | 68.659 | 1.00 30.25 | AAAA |
|--------|------|-----|-------|--------------|--------|--------|-----------|------------|--------|
| MOTA | 2180 | CA | ALA A | | 21.327 | 42.333 | 68.840 | 1.00 29.87 | AAAA |
| | 2181 | CB | ALA A | | 20.005 | 42.119 | 68.112 | 1.00 29.64 | AAAA |
| MOTA | | | | | | | | 1.00 29.35 | |
| MOTA | 2182 | C | ALA A | | 22.395 | 41.438 | 68.247 | | AAAA |
| MOTA | 2183 | 0 | ALA A | | 22.707 | 40.373 | 68.778 | 1.00 29.18 | AAAA |
| MOTA | 2184 | N | PHE A | | 22.946 | 41.893 | 67.127 | 1.00 29.30 | AAAA |
| ATOM | 2185 | CA | PHE A | 275 | 23.991 | 41.170 | 66.428 | 1.00 28.91 | AAAA |
| ATOM | 2186 | CB | PHE A | 275 | 24.375 | 41.909 | 65.150 | 1.00 28.77 | AAAA |
| ATOM | 2187 | CG | PHE A | | 25.354 | 41.170 | 64.308 | 1.00 28.08 | AAAA |
| | 2188 | | PHE A | | 25.015 | 39.954 | 63.740 | 1.00 28.92 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 2189 | | PHE A | | 26.621 | 41.684 | 64.077 | 1.00 29.48 | AAAA |
| MOTA | 2190 | | PHE A | | 25.928 | 39.259 | 62.945 | 1.00 29.20 | AAAA |
| ATOM | 2191 | CE2 | PHE A | 275 | 27.546 | 40.988 | 63.279 | 1.00 29.24 | AAAA |
| MOTA | 2192 | CZ | PHE A | 2 7 5 | 27.193 | 39.779 | 62.716 | 1.00 28.30 | AAAA |
| MOTA | 2193 | С | PHE A | 275 | 25.196 | 41.058 | 67.351 | 1.00 27.64 | AAAA |
| ATOM | 2194 | 0 | PHE A | 275 | 25.728 | 39.975 | 67.558 | 1.00 28.65 | AAAA |
| MOTA | 2195 | N | LEU A | | 25,606 | 42.189 | 67.902 | 1.00 26.81 | AAAA |
| | | CA | LEU A | | 26.732 | 42.260 | 68.831 | 1.00 27.38 | AAAA |
| ATOM | 2196 | | | | | | | 1.00 27.53 | |
| MOTA | 2197 | CB | LEU A | | 26.878 | 43.700 | 69.353 | | AAAA |
| ATOM | 2198 | CG | LEU A | | 28.202 | 44.213 | 69.928 | 1.00 26.37 | AAAA |
| MOTA | 2199 | | LEU A | | 27.923 | 45.488 | 70.721 | 1.00 25.71 | AAAA |
| MOTA | 2200 | CD2 | LEU A | 276 | 28.842 | 43.189 | 70.827 | 1.00 27.06 | AAAA |
| MOTA | 2201 | С | LEU A | 276 | 26.486 | 41.317 | 70.021 | 1.00 26.49 | AAAA |
| ATOM | 2202 | 0 | LEU A | 276 | 27.387 | 40.603 | 70.471 | 1.00 25.26 | AAAA |
| ATOM . | 2203 | N | LYS A | | 25.257 | 41.322 | 70.524 | 1.00 27.46 | AAAA |
| | 2204 | CA | LYS A | | 24.894 | 40.468 | 71.642 | 1.00 28.63 | AAAA |
| MOTA | | | LYS A | | 23.542 | 40.862 | 72.223 | 1.00 30.63 | AAAA |
| MOTA | 2205 | CB | | | | | | | |
| ATOM | 2206 | CG | LYS A | | 23.590 | 42.029 | 73.153 | 1.00 33.14 | AAAA |
| ATOM | 2207 | CD | LYS A | | 22.599 | 41.791 | 74.268 | 1.00 34.94 | AAAA |
| ATOM | 2208 | CE | LYS A | | 22.964 | 40.519 | 75.029 | 1.00 36.17 | AAAA |
| ATOM | 2209 | NZ | LYS A | 277 | 21.979 | 40.194 | 76.104 | 1.00 38.64 | AAAA |
| ATOM | 2210 | С | LYS A | 277 | 24.846 | 38.997 | 71.297 | 1.00 28.53 | AAAA |
| ATOM | 2211 | 0 | LYS A | 27 7 | 25.118 | 38.152 | 72.146 | 1.00 28.45 | AAAA |
| ATOM | 2212 | N | ALA A | 278 | 24.466 | 38.681 | 70.064 | 1.00 28.47 | AAAA |
| | 2213 | CA | ALA A | | 24.404 | 37.280 | 69.656 | 1.00 27.66 | AAAA |
| MOTA | | CB | ALA A | | 23.941 | 37.181 | 68.201 | 1.00 26.40 | AAAA |
| MOTA | 2214 | | | | 25.833 | 36.754 | 69.820 | 1.00 26.63 | AAAA |
| ATOM | 2215 | C | ALA A | | | | | | |
| MOTA | 2216 | 0 | ALA A | | 26.081 | 35.644 | 70.317 | 1.00 25.19 | AAAA |
| MOTA | 2217 | N | PHE A | | 26.764 | 37.616 | 69.427 | 1.00 26.50 | AAAA |
| MOTA | 2218 | CA | PHE A | | 28.181 | 37.345 | 69.481 | 1.00 25.83 | AAAA |
| ATOM | 2219 | CB | PHE A | 279 | 28.934 | 38.521 | 68.869 | 1.00 26.35 | AAAA |
| ATOM | 2220 | CG | PHE A | 279 | 30.413 | 38.319 | 68.796 | 1.00 27.92 | AAAA |
| ATOM | 2221 | CD1 | PHE A | 279 | 30.949 | 37.256 | 68.072 | 1.00 28.58 | AAAA |
| ATOM | 2222 | CD2 | PHE A | 279 | 31.280 | 39.201 | 69.434 | 1.00 28.33 | AAAA |
| ATOM | 2223 | | PHE A | | 32.330 | 37.078 | 67.983 | 1.00 28.22 | AAAA |
| ATOM | 2224 | | PHE A | | 32.666 | 39.030 | 69.349 | 1.00 28.11 | AAAA |
| | | cz | PHE A | | 33.185 | 37.968 | 68.622 | 1.00 28.21 | AAAA |
| MOTA | 2225 | | PHE A | | | 37.118 | 70.901 | 1.00 25.47 | AAAA |
| ATOM | 2226 | C . | | | 28.665 | | | • | |
| Mota | 2227 | 0 | PHE A | | 29.284 | 36.091 | 71.202 | 1.00 24.32 | AAAA |
| MOTA | 2228 | N | ASN A | | 28.382 | 38.075 | 71.778 | 1.00 25.12 | AAAA |
| MOTA | 2229 | CA | ASN A | | | 37.944 | 73.147 | 1.00 25.05 | AAAA |
| ATOM | 2230 | CB | ASN A | 280 | 28.708 | 39.269 | 73.887 | 1.00 24.42 | AAAA |
| ATOM | 2231 | CG | ASN A | 280 | 29.683 | 40.300 | 73.364 | 1.00 24.56 | AAAA |
| MOTA | 2232 | | ASN A | | 30.841 | 39.980 | 73.080 | 1.00 23.24 | AAAA |
| | 2233 | | ASN A | | 29.233 | 41.543 | 73.249 | 1.00 24.59 | AAAA |
| ATOM | | C | ASN A | | 28.213 | 36.814 | 73.925 | 1.00 24.79 | AAAA |
| ATCM | 2234 | | | | | 36.272 | 74.825 | 1.00 24.96 | AAAA |
| MOTA | 2235 | 0 | ASN A | | 28.828 | | | 1.00 24.87 | |
| MOTA | 2236 | N | ILE A | | 26.998 | 36.444 | 73.565 | | AAAA |
| ATOM | 2237 | CA | ILE A | | 26.332 | 35.337 | 74.220 | 1.00 24.80 | AAAA |
| MOTA | 2238 | CB | ILE A | | 24.866 | 35.252 | 73.780 | 1.00 24.40 | AAAA |
| MOTA | 2239 | CG2 | ILE A | 281 | 24.297 | 33.907 | 74.124 | 1.00 25.03 | AAAA |
| ATOM | 2240 | | ILE A | | 24.076 | 36.386 | 74.424 | 1.00 24.70 | AAAA |
| ATOM | 2241 | | ILE A | | 22.613 | 36.379 | 74.069 | 1.00 26.49 | AAAA |
| ATOM | 2242 | c | ILE A | | 27.044 | 34.027 | 73.884 | 1.00 25.21 | AAAA |
| | | ·õ | ILE A | | 27.220 | 33.170 | 74.750 | 1.00 24.97 | AAAA |
| ATOM | 2243 | N | VAL A | | | 33.866 | 72.620 | 1.00 25.98 | AAAA |
| ATCM | 2244 | TA | AWR W | 4- U 4- | 27.440 | JJ.000 | , 2 . 020 | 43.30 | - Lune |

| | | | | | | • | | | | | |
|--------------|--------------|---------|------------|---|------------|---|------------------|------------------|------------------|--------------------------|--------------|
| MOTA | 2245 | CA | VAL | A | 282 | | 28.150 | 32.656 | 72.193 | 1.00 25.15 | AAAA |
| ATOM | 2246 | CB | VAL | Α | 282 | | 28.451 | 32.666 | 70.677 | 1.00 23.83 | AAAA |
| MOTA | 2247 | | VAL | | | | 29.315 | 31.470 | 70.311 | 1.00 23.58 | AAAA |
| MOTA | 2248 | | VAL | | | | 27.173 | 32.633 | 69.899 | 1.00 22.73 | AAAA |
| MOTA | 2249 | C | VAL | | | | 29.478 | 32.553 | 72.936 | 1.00 25.73 | AAAA |
| MOTA | 2250 | 0 | VAL | | | | 29.928 | 31.457 | 73.275 | 1.00 25.31 | AAAA |
| MOTA | 2251 | N | ARG | | | | 30.100 | 33.702 | 73.176 73.885 | 1.00 26.90 1.00 28.87 | AAAA |
| MOTA | 2252 | CA | ARG | | | | 31.372 | 33.760 | 73.684 | 1.00 28.16 | AAAA |
| ATOM | 2253 | CB | ARG | | | | 32.027 32.364 | 35.131 35.440 | 72.240 | 1.00 27.22 | AAAA AAAA |
| ATOM | 2254 | CD. | ARG | | 283 | | 32.821 | 36.862 | 72.098 | 1.00 27.08 | AAAA |
| ATOM | 2255 2256 | NE | | | 283 | | 34.035 | 37.116 | 72.854 | 1.00 26.73 | AAAA |
| ATOM - | 2257 | CZ | ARG | | | | 34.514 | 38.327 | 73.091 | 1.00 26.82 | AAAA |
| ATOM | 2258 | | ARG | | | | 33.873 | 39.384 | 72.626 | 1.00 27.36 | AAAA |
| ATOM | 2259 | | ARG | | | | 35.622 | 38.484 | 73.798 | 1.00 26.95 | AAAA |
| ATOM | 2260 | С | ARG | | | | 31.183 | 33.494 | 75.376 | 1.00 30.71 | AAAA |
| ATOM | 2261 | 0 | ARG | A | 283 | | 32.086 | 32.981 | 76.027 | 1.00 30.68 | AAAA |
| ATOM | 2262 | N | GLU | A | 284 | • | 30.014 | 33.842 | 75.911 | 1.00 32.71 | AAAA |
| ATOM | 2263 | CA | GLU | | | | 29.735 | 33.623 | 77.323 | 1.00 35.53 | AAAA |
| ATOM | 2264 | CB | | | 284 | | 28.482 | 34.391 | 77.751 | 1.00 37.39 | AAAA |
| ATOM | 2265 | CG . | | | 284 | | 28.538 | 35.854 | 77.392 | 1.00 41.73 1.00 45.27 | AAAA |
| ATOM | 2266 | CD | | | 284 | | 27.272 | 36.631 36.078 | 77.754 77.610 | 1.00 45.27 | AAAA AAAA |
| ATOM | 2267 | | GLU GLU | | | | 26.151 27.405 | 37.817 | 78.148 | 1.00 46.94 | AAAA |
| MOTA | 2268 2269 | C | | | 284 | | 29.524 | 32.133 | 77.564 | 1.00 36.25 | AAAA |
| ATOM ATOM | 2270 | 0 | | | 284 | | 29.920 | 31.593 | 78.601 | 1.00 37.85 | AAAA |
| MOTA | 2271 | N | | | 285 | | 28.916 | 31.464 | 76.591 | 1.00 35.24 | AAAA |
| ATOM | 2272 | CA | | | 285 | | 28.637 | 30.041 | 76.708 | 1.00 33.88 | AAAA |
| ATOM | 2273 | CB | VAL | A | 285 | | 27.505 | 29.619 | 75.737 | 1.00 33.71 | AAAA |
| ATOM | 2274 | | VAL | | | | 27.201 | 28.137 | 75.888 | 1.00 32.59 | AAAA |
| ATOM | 2275 | - | VAL | | | | 26.254 | 30.457 | 76.001 | 1.00 32.77 | AAAA |
| ATOM | 2276 | C | | | 285 | | 29.847 | 29.149 | 76.456 | 1.00 33.47 | AAAA |
| MOTA | 2277 | 0 | | | 285 | | 30.140 | 28.262 29.389 | 77.257 75.364 | 1.00 34.23 1.00 32.34 | AAAA AAAA |
| ATOM | 2278 | N CA | | | 286 286 | | 30.568 31.706 | 28.535 | 75.036 | 1.00 32.34 | AAAA |
| ATOM | 2279 2280 | CB | | | 286 | | 31.533 | 27.960 | 73.635 | 1.00 29.77 | AAAA |
| ATOM ATOM | 2281 | CG | | | 286 | | 30.267 | 27.179 | 73.444 | 1.00 28.64 | AAAA |
| ATOM | 2282 | | PHE | | | | 29.152 | 27.772 | 72.863 | 1.00 28.75 | AAAA |
| ATOM | 2283 | | PHE | | | | 30.197 | 25.837 | 73.827 | 1.00 28.55 | AAAA |
| ATOM | 2284 | CE1 | PHE | Α | 286 | | 27.983 | 27.039 | 72.660 | 1.00 29.04 | AAAA |
| MOTA | 2285 | CE2 | PHE | | | | 29.037 | 25.095 | 73.629 | 1.00 28.19 | AAAA |
| MOTA | 2286 | CZ | | | 286 | | 27.929 | 25.694 | 73.045 | 1.00 28.73 | AAAA |
| MOTA | 2287 | C | | | 286 | | 33.106 | 29.113 | 75.132 74.760 | 1.00 29.13 1.00 28.54 | AAAA AAAA |
| MOTA | 2288 | 0 | | | 286 | | 34.073 33.224 | 28.436 30.341 | 75.637 | 1.00 28.42 | AAAA |
| ATOM | 2289 | N CA | | | 287 287 | | 34.525 | 30.987 | 75.744 | 1.00 27.07 | AAAA |
| ATOM | 2290 2291 | C | | | 287 | | 34.932 | 31.611 | 74.419 | 1.00 26.64 | AAAA |
| ATOM ATOM | 2292 | ō | | | 287 | | 34.088 | 32.042 | 73.649 | 1.00 27.13 | AAAA |
| ATOM | 2293 | N | | | 288 | | 36.227 | 31,665 | 74.146 | 1.00 27.20 | AAAA |
| ATOM | 2294 | CA | GLU | A | 288 | | 36.719 | 32.238 | 72.900 | 1.00 27.52 | AAAA |
| MOTA | 2295 | CB | GLU | A | 288 | | 38.073 | 32.923 | 73.108 | 1.00 28.18 | AAAA |
| MOTA | 2296 | CG | | | 288 | | 38.036 | 34.177 | 73.959 | 1.00 28.88 | AAAA |
| MOTA | 2297 | CD | | | 288 | | 37.329 | 35.330 | 73.279 | 1.00 29.58 | AAAA |
| MOTA | 2298 | | GLU | | | | 37.807 | 35.813 | 72.243 73.782 | 1.00 29.94 1.00 31.89 | AAAA AAAA |
| ATOM | 2299 | | GLU | | | | 36.281 | 35.761 | 71.843 | 1.00 31.89 | AAAA |
| ATOM | 2300 | C | | | 288 | | 36.877 | 31.158 30.007 | 72.162 | 1.00 27.87 | AAAA |
| ATOM | 2301 | O M | | | 288 289 | | 37.169 36.663 | 31.547 | 70.589 | 1.00 26.55 | AAAA |
| MOTA | 2302 | N CA | | | 289 | | 36.795 | 30.638 | 69.466 | 1.00 25.25 | AAAA |
| MOTA | 2303 2304 | C | | | 289 | | 37.285 | 31.414 | 68.254 | 1.00 24.55 | AAAA |
| MOTA MOTA | 2304 | ō | | | 289 | | 37.635 | 32.586 | 68.369 | 1.00 24.40 | AAAA |
| ATOM | 2306 | И | | | 290 | | 37.320 | 30.765 | 67.095 | 1.00 24.04 | AAAA |
| ATOM | 2307 | CA | VAL | A | 290 | | 37.756 | 3 1.407 | 65.863 | 1.00 23.76 | AAAA |
| ATOM | 2308 | CB | | | 290 | | 38.288 | 30.346 | 64.867 | 1.00 24.94 | AAAA |
| MOTA | 2309 | | VAL | | | | 38.835 | 31.012 | 63.596 | 1.00 22.73 | AAAA |
| MOTA | 2310 | CG2 | VAL | A | 290 | | 39.375 | 29.506 | 65.555 | 1.00 24.74 | AAAA |

| | | | | | | | | _ | | | |
|--------|------|------|-----|---|------------|--------|--------|----------|--------|-------|-------------|
| MOTA | 2311 | С | VAL | А | 290 | 36.536 | 32.122 | 65.277 | 1.00 2 | 23.90 | AAAA |
| | 2312 | 0 | VAL | | | 35.497 | 31.502 | 65.100 | 1.00 | 25.15 | AAAA |
| ATOM | | | TYR | | | | 33.415 | 64.976 | 1.00 | | AAAA |
| MOTA | 2313 | N | | | | 36.662 | | | | | |
| ATOM | 2314 | CA | TYR | Α | 291 | 35.544 | 34.211 | 64.446 | 1.00 | | AAAA |
| MOTA | 2315 | CB | TYR | Α | 291 | 35.472 | 35.540 | 65.193 | 1.00 | 20.57 | AAAA |
| ATOM | 2316 | CG | TYR | А | 291 | 35.511 | 35:346 | 66.677 | 1.00 | 19.87 | AAAA |
| | | CD1 | | | | 36.596 | 35.782 | 67.432 | 1.00 | | AAAA |
| atom | 2317 | | - | | | | | | | | |
| MOTA | 2318 | CEI | TYR | A | 291 | 36.677 | 35.513 | 68.793 | 1.00 | | AAAA |
| ATOM | 2319 | CD2 | TYR | A | 291 | 34.509 | 34:647 | 67.318 | 1.00 | 20.90 | AAAA |
| | 2320 | | TYR | | | 34.579 | 34.372 | 68.675 | 1.00 | 21.90 | AAAA |
| MOTA | | | | | | | 34.800 | 69.403 | 1.00 | | AAAA |
| ATOM | 2321 | CZ | TYR | | | 35.661 | | | | | |
| MOTA | 2322 | OH | TYR | Α | 291 | 35.737 | 34.469 | 70.730 | 1.00 | | AAAA |
| ATOM | 2323 | С | TYR | A | 291 | 35.607 | 34.483 | 62.946 | 1.00 | 21.25 | AAAA |
| ATOM | 2324 | 0 | TYR | А | 291 | 36.573 | 35.077 | 62.451 | 1.00 | 21.10 | AAAA |
| | | N | LEU | | | 34.557 | 34.084 | 62.231 | 1.00 | | AAAA |
| ATOM | 2325 | | | | | | | | 1.00 | | AAAA |
| ATOM | 2326 | CA | LEU | | | 34.518 | 34.260 | 60.779- | | | |
| MOTA | 2327 | CB | LEU | А | 292 | 34.235 | 32.916 | 60.080 | 1.00 | 19,93 | AAAA |
| ATOM | 2328 | CG | LEU | А | 292 | 35.104 | 31.688 | 60.399 | 1.00 | 17.31 | AAAA |
| | 2329 | | LEU | | | 34.685 | 30.515 | 59.528 | 1.00 | 16.05 | AAAA |
| ATOM | | | | | | | | 60.163 | 1.00 | | AAAA |
| ATOM | 2330 | | LEU | | | 36.552 | 32.000 | | | | |
| MOTA | 2331 | С | LEU | А | 292 | 33.515 | 35.288 | 60.283 | 1.00 | | AAAA |
| MOTA | 2332 | 0 | LEU | Α | 292 | 32.652 | 35.741 | 61.020 | 1.00 | 20.70 | AAAA |
| ATOM | 2333 | N | GLY | А | 293 | 33.660 | 35.660 | 59.017 | 1.00 | 21.74 | AAAA |
| | | CA | GLY | | | 32.752 | 36.612 | 58.410 | 1.00 | 21.48 | AAAA |
| ATOM | 2334 | | | | | | | 57.770 | 1.00 | | AAAA |
| ATOM | 2335 | С | GLY | | - | 31.612 | 35.856 | | | | |
| ATOM | 2336 | 0 | GLY | A | 293 | 31.237 | 34.790 | 58.235 | 1.00 | | AAAA |
| ATOM | 2337 | N | GLY | Α | 294 | 31.060 | 36.392 | 56.691 | 1.00 | 22.66 | AAAA |
| ATOM | 2338 | CA | GLY | A | 294 | 29.957 | 35.714 | 56.034 | 1.00 | 23.61 | AAAA |
| | | | GLY | | | 29.180 | 36.653 | 55.146 | 1.00 | | AAAA |
| MOTA | 2339 | C | | | | | | | | | |
| ATOM - | 2340 | 0 | GLY | | | 29.679 | 37.727 | 54.790 | 1.00 | | AAAA |
| MOTA | 2341 | N | GLY | A | 295 | 27.956 | 36.265 | 54.794 | | 24.06 | AAAA |
| ATOM | 2342 | CA | GLY | Α | 295 | 27.139 | 37.093 | 53.927 | 1.00 | 22.78 | AAAA |
| | 2343 | C | GLY | | | 26.902 | 38.479 | 54.483 | 1.00 | 23.11 | AAAA |
| MOTA | | | | | 295 | 26.870 | 38.676 | 55.696 | | 22.87 | AAAA |
| ATOM | 2344 | 0 | | | | | | | | 22.78 | AAAA |
| ATOM | 2345 | N | GLY | | | 26.733 | 39.442 | 53.584 | | | |
| ATOM | 2346 | CA | | | 296 | 26.497 | 40.813 | 53.993 | | 23.44 | AAAA |
| ATOM | 2347 | С | GLY | A | 296 | 26.471 | 41.618 | 52.718 | 1.00 | 23.72 | AAAA |
| | 2348 | 0 | GLY | | | 27.474 | 41.661 | 52.004 | 1.00 | 23.73 | AAAA |
| ATOM | | | | | 297 | 25.356 | 42.280 | 52.425 | 1.00 | 23.41 | AAAA |
| ATOM | 2349 | N | | | | | | 51.163 | | 22.71 | AAAA |
| MOTA | 2350 | CA | TYR | | | 25.282 | 42.991 | | | | |
| ATOM | 2351 | CB | TYR | A | 297 | 24.252 | 42.294 | | | 21.55 | AAAA |
| MOTA | 2352 | CG | TYR | Α | 297 | 24.496 | 40.809 | 50.317 | 1.00 | 21.93 | AAAA |
| | 2353 | | TYR | Α | 297 | 24.036 | 40.016 | 51.375 | 1.00 | 20.95 | AAAA |
| MOTA | | | TYR | | | 24.400 | 38.678 | 51.481 | 1 00 | 21.59 | AAAA |
| MOTA | 2354 | | | | | | | 49.358 | | 21.71 | AAAA |
| MOTA | 2355 | | TYR | | | 25.320 | 40.217 | | | | |
| ATOM | 2356 | CE2 | TYR | A | 297 | 25.688 | 38.900 | 49.451 | | 21.99 | AAAA |
| ATOM | 2357 | CZ | TYR | Α | 297 | 25.242 | 38.127 | 50.511 | 1.00 | 22.18 | AAAA |
| | 2358 | OH | ጥV₽ | А | 297 | 25.721 | 36.841 | 50.615 | 1.00 | 21.35 | AAAA |
| ATOM | | | | | 297 | 25.042 | 44.485 | 51.225 | | 22.90 | AAAA |
| ATOM | 2359 | С | | | | | | | | | |
| ATOM | 2360 | 0 | | | 297 | 25.106 | 45.172 | 50.203 | | 23.17 | AAAA |
| ATOM | 2361 | N | HIS | A | 298 | 24.772 | 44.989 | 52.417 | | 22.47 | AAAA |
| | 2362 | CA | HIS | Α | 298 | 24.572 | 46.415 | 52.566 | 1.00 | 24.27 | AAAA |
| MOTA | | CB | HIS | | | 23.468 | 46.726 | 53.556 | 1.00 | 23.17 | AAAA |
| ATOM | 2363 | | | | | | 40 166 | . 53.572 | | 23.20 | AAAA |
| ATOM | 2364 | CG | HIS | | | 23.097 | | | | | |
| ATOM | 2365 | CD2 | HIS | A | 298 | 23.588 | 49.201 | 54.287 | 1.00 | 24.25 | AAAA |
| ATOM | 2366 | ND1 | HIS | Α | 298 | 22.199 | 48.708 | 52.680 | | 23.14 | AAAA |
| | 2367 | CFI | HIS | Α | 298 | 22.151 | 50.017 | 52.848 | | 23.31 | AAAA |
| MOTA | | ZEC. | HIS | λ | 298 | 22.986 | 50.342 | 53.814 | | 23.62 | AAAA |
| MOTA | 2368 | | | | | | | | | 25.17 | AAAA |
| MOTA | 2369 | С | | | 298 | 25.886 | 46.976 | 53.106 | | | |
| MOTA | 2370 | 0 | HIS | A | 298 | 26.282 | 46.687 | 54.239 | | 24.47 | AAAA |
| | 2371 | N | | | 299 | 26.563 | 47.818 | 52.316 | 1.00 | 26.37 | AAAA |
| ATOM | | | | | 299 | 26.178 | 48.372 | 51.006 | | 27.01 | AAAA |
| MOTA | 2372 | CD | | | | | | 52.752 | | 27.31 | AAAA |
| ATOM | 2373 | CA | | | 299 | 27.840 | 48.394 | | | | |
| MOTA | 2374 | CB | | | 299 | 28.156 | 49.383 | 51.630 | | 27.04 | AAAA |
| ATOM | 2375 | ÇG | PRO | Α | 299 | 26.743 | 49.764 | 51.120 | | 27.57 | AAAA |
| 2 | 2376 | č | | | 299 | 27.824 | 49.037 | 54.149 | 1.00 | 27.77 | AAAA |
| ATOM | 23/0 | _ | | | | 2 | 23.03/ | | | | |
| | | | | | | | | | • | | |
| | | _ | | | | | | | | | |

| ATOM | 2377 | 0 | PRO | Α | 299 | | 28.755 | 48.826 | 54.939 | 1.00. | 28.04 | AAAA |
|--------|------|-----|--------|----|------|---|--------|--------|----------|-------|-------|-------|
| ATOM | 2378 | N | TYR | Α | 300 | | 26.769 | 49.794 | 54.452 | 1.00 | 27.04 | AAAA |
| ATOM | 2379 | CA | _ | | 300 | | 26.629 | 50.477 | 55.740 | | 27.59 | AAAA |
| | | | | | 300 | | 25.425 | 51.437 | 55.700 | | 30.57 | AAAA |
| MOTA | 2380 | СВ | | | | | | | | | | |
| ATOM | 2381 | CG | | | 300 | | 25.516 | 52.599 | 54.718 | | 32.91 | AAAA |
| ATOM - | 2382 | | | | 300 | | 26.181 | 52.464 | 53.491 | | 33.45 | AAAA |
| MOTA | 2383 | CE1 | TYR | Α | 300 | | 26.160 | 53.487 | 52.538 | 1.00 | 33.91 | AAAA |
| ATOM | 2384 | CD2 | TYR | А | 300 | | 24.837 | 53.801 | 54.969 | 1.00 | 34.19 | AAAA |
| MOTA | 2385 | CE2 | | | 300 | | 24.809 | 54.830 | | | 34.64 | AAAA |
| | | | | | | | 25.468 | 54.657 | 52.807 | | 34.56 | AAAA |
| MOTA | 2386 | CZ | | | 300 | | | | | | | |
| MOTA | 2387 | OH | | | 300 | | 25.389 | 55.630 | 51.844 | | 36.05 | AAAA |
| MOTA | 2388 | С | | | .300 | | 26.454 | 49.538 | 56.936 | | 26.48 | AAAA |
| ATOM | 2389 | 0 | TYR | Α | 300 | - | 27.073 | 49.726 | 57.979 - | 1.00 | 25.81 | AAAA |
| MOTA | 2390 | N | ALA | Α | 301 | | 25.581 | 48.547 | 56.791 | 1.00 | 25.41 | AAAA |
| ATOM | 2391 | CA | | | 301 | | 25.328 | 47.606 | 57.865 | 1.00 | 24.64 | AAAA |
| | 2392 | CB | | | 301 | | 24.164 | 46.731 | 57.511 | | 25.32 | -AAAA |
| MOTA | | | | | | | 26.568 | 46.775 | 58.067 | | 25.53 | AAAA |
| MOTA | 2393 | C | | | 301 | | | | | | | |
| ATOM | 2394 | 0 | | | 301 | | 27.030 | 46.567 | 59.194 | | 26.39 | AAAA |
| MOTA . | 2395 | N | LEU | Α | 302 | | 27.108 | 46.304 | | | 25.83 | AAAA |
| ATOM | 2396 | CA | LEU | Α | 302 | | 28.323 | 45.500 | 56.926 | 1.00 | 26.32 | AAAA |
| ATOM | 2397 | CB | LEU | A | 302 | | 28.782 | 45.378 | 55.479 | 1.00 | 27.38 | AAAA |
| ATOM | 2398 | CG | LEU | Α | 302 | | 30.081 | 44.723 | 55.024 | 1.00 | 28.18 | AAAA |
| ATOM | 2399 | | | | 302 | | 30.119 | 44.840 | 53.502 | | 29.32 | AAAA |
| | 2400 | | | | 302 | | 31.296 | 45.389 | 55.613 | | 27.38 | AAAA |
| ATOM | _ | | | | | | | | | | | |
| MOTA | 2401 | C | | | 302 | | 29.398 | 46.187 | 57.764 | | 26.41 | AAAA |
| ATOM | 2402 | 0 | | | 302 | | 29.874 | 45.648 | 58.755 | | 26.62 | AAAA |
| MOTA | 2403 | N | | | 303 | | 29.756 | 47.397 | 57.353 | | 26.50 | AAAA |
| ATOM | 2404 | CA | ALA | Α | 303 | | 30.778 | 48.176 | 58.022 | 1.00 | 25.92 | AAAA |
| ATOM | 2405 | CB | ALA | Α | 303 | | 31.001 | 49.475 | 57.277 | 1.00 | 25.24 | AAAA |
| MOTA | 2406 | С | ALA | А | 303 | | 30.490 | 48.464 | 59.487 | 1.00 | 26.03 | AAAA |
| | 2407 | ō | | | 303 | | 31.325 | 48.175 | 60.340 | | 26.95 | AAAA |
| ATOM | | | | | 304 | | 29.322 | 49.028 | 59.792 | | 25.29 | AAAA |
| MOTA | 2408 | N | | | | | | | 61.179 | | 23.46 | AAAA |
| MOTA | 2409 | CA | | | 304 | | 28.999 | 49.353 | | | | |
| MOTA | 2410 | CB | - | | 304 | • | 27.641 | 50.059 | 61.291 | | 23.78 | AAAA |
| MOTA | 2411 | CG | | | 304 | | 27.553 | 51.451 | 60,629 | | 24.59 | AAAA |
| ATOM | 2412 | CD | ARG | A | 304 | | 26.302 | 52.223 | 61.091 | 1.00 | 25.85 | AAAA |
| MOTA | 2413 | NE | ARG | A | 304 | | 25.067 | 51.465 | 60.869 | 1.00 | 27.54 | AAAA |
| ATOM | 2414 | CZ | ARG | Α | 304 | | 23.978 | 51.547 | 61.637 | 1.00 | 28.36 | AAAA |
| ATOM | 2415 | | | | 304 | | 23.957 | 52.362 | 62.695 | 1.00 | 26.48 | AAAA |
| | 2416 | | | | 304 | | 22.910 | 50.794 | 61.358 | | 28.45 | AAAA |
| MOTA | | | | | 304 | | 28.991 | 48.118 | 62.053 | | 23.18 | AAAA |
| ATOM | 2417 | C | | | | | | | | | 22.26 | AAAA |
| ATOM | 2418 | 0 | | | 304 | | 29.591 | 48.099 | 63.135 | | | |
| ATOM | 2419 | N | | | 305 | | 28.330 | 47.075 | 61.560 | | 23.20 | AAAA |
| ATOM | 2420 | CA | | | 305 | | 28.200 | 45.817 | 62.292 | | 22.33 | AAAA |
| ATOM | 2421 | CB | ALA | A. | 305 | | 27.319 | 44.866 | 61.516 | 1.00 | 22.17 | AAAA |
| MOTA | 2422 | С | ALA | Α | 305 | | 29.516 | 45.137 | 62.621 | 1.00 | 22.27 | AAAA |
| ATOM | 2423 | ō | | | 305 | | 29.763 | 44.757 | 63.760 | 1.00 | 22.48 | AAAA |
| | 2424 | N | | | 306 | | 30.366 | 44.969 | 61.620 | | 22.57 | AAAA |
| ATOM | 2425 | CA | | _ | 306 | | 31.634 | 44.307 | 61.861 | | 21.28 | AAAA |
| ATOM | | | | | | | | | | | 21.07 | AAAA |
| ATQM | 2426 | CB | | | 306 | | 32.279 | 43.885 | 60.553 | | | |
| ATOM | 2427 | CG | | | 306 | | 31.703 | 42.618 | 60.004 | | 20.75 | AAAA |
| ATOM | 2428 | | TRP | | | | 31.886 | 42.103 | 58.683 | | 19.54 | AAAA |
| ATOM | 2429 | CE2 | TRP | Α | 306 | | 31.352 | 40.795 | 58.668 | 1.00 | 19.18 | AAAA |
| ATOM | 2430 | CE3 | TRP | Α | 306 | | 32.456 | 42.616 | 57.510 | 1.00 | 19.59 | AAAA |
| ATOM | 2431 | | TRP | | | | 31.071 | 41.632 | 60.713 | | 20.51 | AAAA |
| | 2432 | | TRP | | | | 30.864 | 40.537 | 59.922 | | 19.74 | |
| ATOM | | NOT | TVE | 7 | 306 | | 31.368 | 39.990 | 57.524 | | 19.18 | AAAA |
| MOTA | 2433 | | | | | | | | | | | AAAA |
| MOTA | 2434 | CZ3 | TRP | A | 306 | | 32.474 | 41.810 | 56.367 | | 18.98 | |
| MOTA | 2435 | CH2 | TRP | | | | 31.933 | 40.513 | 56.388 | | 19.21 | AAAA |
| ATOM | 2436 | С | TRP | A | 306 | | 32.571 | 45.159 | 62.674 | | 20.80 | AAAA |
| ATOM | 2437 | 0 | TRP | Α | 306 | | 33.459 | 44.630 | 63.341 | | 20.55 | AAAA |
| ATOM | 2438 | N | THR | A | 307 | | 32.373 | 46.475 | 62.614 | 1.00 | 20.17 | AAAA |
| | | CA | מנויוי | Α | 307 | | 33.175 | 47.399 | 63.407 | | 20.54 | AAAA |
| ATOM | 2439 | | | | 307 | | 32.861 | 48.881 | 63.045 | | 21.09 | AAAA |
| MOTA | 2440 | CB | THK | - | 207 | | | | 61 710 | | 21.25 | AAAA |
| ATOM | 2441 | OG1 | THR | A | 30/ | | 33.329 | 49.159 | 61.718 | | | |
| ÄTOM | 2442 | CG2 | THR | A | 307 | | 33.523 | 49.839 | 64.030 | 1.00 | 20.09 | AAAA |
| | | | | | | | | | - | | | • |



| ATOM | 2443 | С | THR A 307 | 32.853 | 47.135 | 64.893 | 1.00 20.88 | AAAA |
|------|-------|-----|-----------|--------|---------|--------|------------|--------|
| ATOM | 2444 | ō | THR A 307 | 33.738 | 47.175 | 65.747 | 1.00 21.89 | AAAA |
| | | N | LEU A 308 | 31.588 | 46.851 | 65.192 | 1.00 20.10 | AAAA |
| ATOM | 2445 | | | | 46.543 | 66.559 | 1.00 21.10 | AAAA |
| MOTA | 2446 | | LEU A 308 | 31.189 | | 66.644 | 1.00 20.99 | AAAA |
| MOTA | 2447 | CB | LEU A 308 | 29.671 | 46.340 | | | |
| MOTA | 2448 | CG | LEU A 308 | 28.897 | 47.656 | 66.674 | 1.00 21.54 | AAAA |
| MOTA | 2449 | CD1 | LEU A 308 | 27.397 | 47.473 | 66.411 | 1.00 19.91 | AAAA |
| ATOM | 2450 | CD2 | LEU A 308 | 29.177 | 48.283 | 68.045 | 1.00 21.04 | AAAA |
| ATOM | 2451 | С | LEU A 308 | 31.886 | 45.284 | 67.052 | 1.00 21.98 | AAAA |
| ATOM | 2452 | ō | LEU A 308 | 32.284 | 45.186 | 68.215 | 1.00 22.17 | AAAA |
| | 2453 | Ŋ | ILE A 309 | 32.023 | 44.310 | 66.165 | 1.00 22:32 | AAAA |
| ATOM | | | ILE A 309 | 32.658 | 43.069 | 66.544 | 1.00 23.12 | AAAA |
| ATOM | 2454 | CA | | | 42.016 | 65.413 | 1.00 22.33 | AAAA · |
| MOTA | 2455 | CB | ILE A 309 | 32.590 | | 65.827 | 1.00 21.76 | AAAA |
| MOTA | 2456 | | ILE A 309 | 33.356 | 40.787 | | | AAAA |
| MOTA | 2457 | | ILE A 309 | 31.140 | 41.678 | 65.061 | 1.00 22.16 | |
| MOTA | 2458 | CD1 | ILE A 309 | 30.366 | 41.037 | 66.166 | 1.00 22.01 | AAAA |
| MOTA | 2459 | С | ILE A 309 | 34.115 | 43.377 | 66.790 | 1.00 24.52 | AAAA |
| ATOM | 2460 | 0 | ILE A 309 | 34.734 | 42.828 | 67.709 | 1.00 25.72 | AAAA |
| ATOM | 2461 | N | TRP A 310 | 34.673 | 44.253 | 65.957 | 1.00 24.70 | AAAA |
| MOTA | 2462 | CA | TRP A 310 | 36.075 | 44.570 | 66.099 | 1.00 24.20 | AAAA |
| | 2463 | CB | TRP A 310 | 36.587 | 45.417 | 64.944 | 1.00 23.29 | AAAA |
| ATOM | | | TRP A 310 | 38.040 | 45.712 | 65.123 | 1.00 23.17 | AAAA |
| MOTA | 2464 | CG | | 39.104 | 44.752 | 65.257 | 1.00 21.36 | AAAA |
| MOTA | 2465 | CD2 | | | | 65.490 | 1.00 20.62 | AAAA |
| MOTA | 2466 | | TRP A 310 | 40.291 | 45.472 | | 1.00 20.01 | AAAA |
| MOTA | 2467 | | TRP A 310 | 39.165 | 43.354 | 65.202 | - | |
| MOTA | 2468 | | TRP A 310 | 38.614 | 46.93B | 65.273 | 1.00 22.82 | AAAA |
| MOTA | 2469 | NE1 | TRP A 310 | 39.967 | 46.803 | 65.497 | 1.00 22.30 | AAAA |
| MOTA | 2470 | CZ2 | TRP A 310 | 41.521 | 44.845 | 65.668 | 1.00 19.91 | AAAA |
| MOTA | 2471 | CZ3 | TRP A 310 | 40.388 | 42.734 | 65.381 | 1.00 19.08 | AAAA |
| ATOM | 2472 | CH2 | TRP A 310 | 41.547 | 43.477 | 65.610 | 1.00 19.40 | AAAA |
| MOTA | 2473 | C | TRP A 310 | 36.318 | 45.279 | 67.411 | 1.00 25.26 | AAAA |
| ATOM | 2474 | ŏ | TRP A 310 | 37.262 | 44.945 | 68.109 | 1.00 24.71 | AAAA |
| | 2475 | N | CYS A 311 | 35.467 | 46.247. | | 1.00 26.76 | AAAA |
| MOTA | 2476 | CA | CYS A 311 | 35.608 | 46.975 | 69.007 | 1.00 27.89 | AAAA |
| MOTA | | | CYS A 311 | 34:548 | 48.081 | 69.113 | 1.00 28.98 | AAAA |
| MOTA | .2477 | CB | | 34.798 | 49.462 | 67.991 | 1.00 31.89 | AAAA |
| ATOM | 2478 | SG | CYS A 311 | 35.495 | 46.043 | 70.212 | 1.00 27.51 | AAAA |
| ATOM | 2479 | C | CYS A 311 | | 46.127 | 71.135 | 1.00 26.90 | AAAA |
| MOTA | 2480 | 0 | CYS A 311 | 36.289 | | | 1.00 27.33 | AAAA |
| MOTA | 2481 | N | GLU A 312 | 34.495 | 45.169 | 70.187 | 1.00 28.03 | AAAA |
| ATOM | 2482 | CA | GLU A 312 | 34.246 | 44.210 | 71.250 | | |
| MOTA | 2483 | CB | GLU A 312 | 33.106 | 43.287 | 70.850 | 1.00 28.55 | AAAA |
| MOTA | 2484 | CG | GLU A 312 | 31.903 | 43.333 | 71.741 | 1.00 28.93 | AAAA |
| ATOM | 2485 | CD | GLU A 312 | 32.232 | 42.958 | 73.154 | 1.00 29.78 | AAAA |
| ATOM | 2486 | 0E1 | GLU A 312 | 32.954 | 41.957 | 73.345 | 1.00 30.81 | AAAA |
| ATOM | 2487 | OE2 | GLU A 312 | 31.754 | 43.653 | 74.071 | 1.00 30.79 | AAAA |
| ATOM | 2488 | c | GLU A 312 | 35.463 | 43.357 | 71 514 | 1.00 28.91 | AAAA |
| ATOM | 2489 | ō | GLU A 312 | 35.822 | 43.110 | 72 662 | 1.00 30.57 | AAAA |
| | 2490 | N | LEU A 313 | 36.081 | 42.889 | 70.436 | 1.00 29.04 | AAAA |
| ATOM | 2491 | CA | LEU A 313 | 37.266 | 42.045 | 70.516 | 1.00 28.87 | AAAA |
| MOTA | | | LEU A 313 | 37.524 | 41.373 | 69.157 | 1.00 29.39 | AAAA |
| MOTA | 2492 | CB | | | 40.311 | 68.644 | 1.00 30.32 | AAAA |
| ATOM | 2493 | CG | LEU A 313 | 36.548 | | 67.215 | 1.00 30.26 | AAAA |
| ATOM | 2494 | | LEU A 313 | 36.910 | 39.872 | | 1.00 30.42 | AAAA |
| MOTA | 2495 | CD2 | LEU A 313 | 36.582 | 39.114 | 69.593 | 1.00 30.42 | |
| ATOM | 2496 | С | LEU A 313 | 38.474 | 42.888 | 70.905 | | AAAA |
| ATOM | 2497 | 0 | LEU A 313 | 39.215 | 42.553 | 71.808 | 1.00 27.34 | AAAA |
| ATOM | 2498 | N | SER A 314 | 38.642 | 43.986 | 70.191 | 1.00 27.95 | AAAA |
| ATOM | 2499 | CA | SER A 314 | 39.736 | 44.927 | 70.376 | | AAAA |
| ATOM | 2500 | CB | SER A 314 | 39.690 | 45.937 | 69.231 | 1.00 27.49 | AAAA |
| | 2501 | OG | SER A 314 | 40.703 | 46.904 | 69.343 | 1.00 30.12 | AAAA |
| ATOM | | C | SER A 314 | 39.666 | 45.653 | | 1.00 29.67 | AAAA |
| ATOM | 2502 | | SER A 314 | 40.488 | 46.517 | 72.023 | 1.00 29.00 | AAAA |
| ATOM | 2503 | 0 | GLY A 315 | 38.676 | 45.302 | 72.538 | | AAAA |
| MOTA | 2504 | N | CIV X 315 | | | 73.827 | | AAAA |
| MOTA | 2505 | CA | GLY A 315 | 38.535 | 45.935 | | | AAAA |
| MOTA | 2506 | С | GLY A 315 | 38.542 | 47.452 | | · | AAAA |
| ATOM | 2507 | 0 | GLY A 315 | 39.142 | 48.091 | 74.647 | | |
| MOTA | 2508 | N | ARG A 316 | 37.881 | 48.041 | 72.794 | 1.00 36.88 | AAAA. |

| ATOM | 2509 | CA | ARG A | 316 | 37.841 | 49.493 | 72.702 | 1.00 | 39.49 | AAAA |
|--------|--------------|-----|----------|-----|--------|--------|--------|------|--------------|------|
| MOTA | 2510 | CB | ARG A | 316 | 38.608 | 49.968 | 71.484 | | 39.86 | AAAA |
| ATOM | 2511 | CG | ARG A | 316 | 37.946 | 49.677 | 70.161 | _ | 40.77 | AAAA |
| MOTA | 2512 | CD | ARG A | | 38.843 | 50.226 | 69.077 | | 41.47 | AAAA |
| MOTA | 2513 | NE | ARG A | | 40.140 | 49.566 | 69.092 | _ | 42.36 | AAAA |
| ATOM | 2514 | CZ | ARG A | | 41.224 | 50.057 | 68.515 | | 43.38 | AAAA |
| MOTA | 2515 | | ARG A | | 41.159 | 51.217 | 67.882 | | 44.76 | |
| MOTA | 2516 | | ARG A | | 42.361 | 49.385 | 68.556 | | 43.71 | AAAA |
| ATOM | 2517 | С | ARG A | | 36.418 | 50.015 | 72.631 | | | AAAA |
| MOTA | 2518 | ō | ARG A | | 35.564 | | | | 41.54 | AAAA |
| ATOM | 2519 | Ŋ | GLU A 3 | | 36.163 | 49.429 | 71.959 | | 42.64 | AAAA |
| | 2520 | CA | GLU A 3 | | | 51.119 | 73.329 | | 43.10 | AAAA |
| MOTA | | CB | GLU A 3 | | 34.830 | 51.720 | 73.356 | | 44.51 | AAAA |
| ATOM | 2521 2522 | CG | GLU A 3 | | 34.809 | 52.936 | 74.293 | | 46.17 | AAAA |
| ATOM | | CD | | | 34.472 | 52.614 | 75.759 | | 49.65 | AAAA |
| ATOM | 2523 | | GLU A 3 | | 35.426 | 51.623 | 76.439 | | 52.51 | AAAA |
| ATOM | 2524 | | _ | _ | 35.153 | 51.251 | 77.607 | | 53.37 | AAAA |
| ATOM | 2525 | | GLU A 3 | | 36.444 | 51.214 | 75.831 | | 54.14 | AAAA |
| ATOM | 2526 | C | GLU A 3 | | 34.318 | 52.098 | 71.974 | | 43.86 | AAAA |
| ATOM | 2527 | 0 | GLU A 3 | | 35.067 | 52.532 | 71.108 | | 42.46 | AAAA |
| ATOM | 2528 | N | VAL A 3 | | 33.023 | 51.916 | 71.779 | | 44.79 | AAAA |
| ATOM | 2529 | CA | VAL A 3 | | 32.394 | 52.197 | 70.502 | | 45.57 | AAAA |
| MOTA | 2530 | CB | VAL A 3 | | 31.098 | 51.369 | 70.324 | | 45.36 | AAAA |
| ATOM | 2531 | | VAL A 3 | | 30.537 | | 68.924 | | 45.44 | AAAA |
| MOTA | 2532 | | VAL A 3 | | 31.366 | 49.911 | 70.612 | | 46.35 | AAAA |
| MOTA | 2533 | C | VAL A 3 | | 32.007 | 53.652 | 70.377 | 1.00 | 46.41 | AAAA |
| ATOM | 2534 | 0 | VAL A 3 | | 31.199 | 54.145 | 71.165 | 1.00 | 46.53 | AAAA |
| MOTA | 2535 | N | PRO A 3 | | 32.584 | 54.370 | 69.396 | | 46.89 | AAAA |
| MOTA | 2536 | CD | PRO A 3 | | 33.581 | 54.017 | 68.375 | | 46.44 | AAAA |
| ATOM | 2537 | | PRO A 3 | | 32.209 | 55.774 | 69.247 | | 47.62 | AAAA |
| MOTA | 2538 | CB | PRO A 3 | | 33.022 | 56.206 | 68.024 | | 46.96 | AAAA |
| ATOM | 2539 | CG | PRO A 3 | | 33.161 | 54.922 | 67.251 | | 46.38 | AAAA |
| ATOM | 2540 | C | PRO A 3 | | 30.709 | 55.743 | 68.977 | 1.00 | 48.64 | AAAA |
| MOTA | 2541 | 0 | PRO A 3 | | 30.236 | 54.860 | 68.262 | 1.00 | 48.61 | AAAA |
| MOTA | 2542 | N | GLU A 3 | | 29.944 | 56.667 | 69.544 | | 49.24 | AAAA |
| MOTA | 2543 | CA | GLU A 3 | | 28.522 | 56.598 | 69.288 | | 50.01 | AAAA |
| ATOM | 2544 | CB | GLU A 3 | | 27.720 | 57.330 | 70.363 | | 51.15 | AAAA |
| MOTA | 2545 | CG | GLU A 3 | | 27.828 | 58.831 | 70.339 | | 53.01 | AAAA |
| MOTA | 2546 | CD | GLU A 3 | | 26.825 | 59.474 | 71.282 | | 54.34 | AAAA |
| MOTA | 2547 | | GLU A 3 | | 25.604 | 59.273 | 71.077 | | 54.04 | AAAA |
| MOTA | 2548 | | GLU A 3 | | 27.255 | 60.171 | 72.228 | | 55.06 | AAAA |
| ATOM | 2549 | C | GLU A 3 | | 28.206 | 57.168 | 67.921 | | 49.78 | AAAA |
| MOTA | 2550 | 0 | GLU A 3 | | 27.170 | 56.861 | 67.324 | | 49.79 | AAAA |
| MOTA | 2551 | N | LYS A 3 | | 29.116 | 57.980 | 67.407 | | 49.26 | AAAA |
| ATOM | 2552 | CA | LYS A 3 | | 28.906 | 58.589 | 66.109 | | 49.20 | AAAA |
| ATOM | 2553 | CB | LYS A 3 | | 28.873 | 60.106 | 66.251 | | 50.38 | AAAA |
| MOTA | > 354 | CG | LYS A 3 | | 30.234 | 60.674 | 66.634 | | 52.88 | AAAA |
| ATOM | 555 | CD | LYS A 3 | | 30.717 | 60.180 | 68.002 | | 53.76 | AAAA |
| ATOM | 2356 | CE | LYS A 3 | | 32.229 | 60.348 | 68.154 | | 55.00 | AAAA |
| MOTA | 2557 | NZ | LYS A 3 | | 32.715 | 61.725 | 67.829 | | 55.95 | AAAA |
| ATOM | 2558 | Ç | LYS A 3 | | 30.037 | 58.207 | 65.171 | | 48.64 | AAAA |
| ATOM | 2559 | Ο. | LYS A 3 | | 31.052 | 57.650 | 65.590 | | 48.58 | AAAA |
| ATOM | 2560 | N | LEU A 3 | | 29.854 | 58.511 | 63.894 | | 47.78 | AAAA |
| MOTA | 2561 | CA | LEU A 3 | | 30.870 | 58.238 | 62.896 | | 46.13 | AAAA |
| ATOM | 2562 | CB | LEU A 3 | | 30.248 | 57.638 | 61.638 | 1.00 | 46.84 | AAAA |
| MOTA | 2563 | CG | LEU A 32 | | 29.240 | 56.504 | 61.848 | 1.00 | 47.71 | AAAA |
| MOTA | 2564 | | LEU A 3 | | 28.788 | 55.998 | 60.491 | 1.00 | 48.02 | AAAA |
| MOTA | 25,65 | | LEU A 32 | | 29.853 | 55.374 | 62.667 | 1.00 | | AAAA |
| ATOM | 2566 | | LEU A 32 | | 31.427 | 59.608 | 62.580 | 1.00 | 44.61 | AAAA |
| MOTA | 2567 | | LEU A 32 | | 30.674 | 60.571 | 62.491 | 1.00 | | AAAA |
| ATOM | 2568 | N | ASN A 32 | 23 | 32.741 | 59.706 | 62.447 | | 42.66 | AAAA |
| ATOM | 2569 | CA | ASN A 32 | 23 | 33.360 | 60.976 | 62.135 | 1.00 | | AAAA |
| ATOM | 2570 | | ASN A 32 | | 34.860 | 60.904 | 62.402 | | 41.07 | AAAA |
| ATOM | 2571 | CG | ASN A 32 | 23 | 35.576 | 60.001 | 61.436 | 1.00 | | AAAA |
| ATOM · | 2572 | OD1 | ASN A 32 | 23 | 35.117 | 58.901 | 61.147 | | 42.46 | AAAA |
| ATOM | 2573 | ND2 | ASN A 32 | 23 | 36.720 | 60.449 | 60.943 | 1.00 | | AAAA |
| ATOM | 2574 | | ASN A 32 | | 33.068 | 61.223 | | | 40.76 | AAAA |
| | | ٠. | | | | | | | - | |

SUBSTITUTE SHEET (RULE 26)

| ATOM | 2575 | Ο. | ASN A | 323 | 32.430 | 60.395 | 60.010 | 1.00 40.19 | AAAA |
|------|--------|------|-------|-------|----------|--------|--------|------------|--------|
| ATOM | 2576 | N | ASN A | 324 | 33.523 | 62.352 | 60.129 | 1.00 40.11 | AAAA |
| | | | | | | | | | |
| ATOM | 2577 | CA | ASN A | | 33.268 | 62.699 | 58.735 | 1.00 39.99 | AAAA |
| ATOM | 2578 | CB | ASN A | 324 | 33.711 | 64.128 | 58.472 | 1.00 39.54 | AAAA |
| ATOM | 2579 | CG | ASN A | 324 | 33.003 | 65.114 | 59.361 | 1.00 40.88 | AAAA |
| | | | | | | | | | |
| ATOM | 2580 | | ASN A | | 31.763 | 65.145 | 59.417 | 1.00 40.77 | AAAA |
| ATOM | 2581 | ND2 | ASN A | 324 | 33.779 | 65.938 | 60.064 | 1.00 40.63 | AAAA |
| | 2582 | c - | ASN A | | | 61.786 | 57.712 | 1.00 40.10 | AAAA |
| MOTA | | | | | | | | | |
| MOTA | 2583 | 0 | ASN A | 324 | 33.320 | 61.468 | 56.678 | 1.00 39.24 | AAAA |
| MOTA | 2584 | N | LYS A | 325 | 35.144 | 61.376 | 58.011 | 1.00 40.41 | AAAA |
| | | CA | LYS A | | | 60.519 | 57.126 | 1.00 41.41 | AAAA |
| MOTA | 2585 | | | | | | | | |
| MOTA | 2586 | CB | LYS A | . 325 | 37.262 | 60.201 | 57.761 | 1.00 42.64 | , AAAA |
| ATOM | 2587 | CG | LYS A | 325 | 38.224 | 59.504 | 56.828 | 1.00 44.45 | AAAA |
| | | CD | LYS A | | 39.575 | 59.199 | 57.491 | 1.00 45.61 | AAAA |
| MOTA | 2588 | | | | | | | | |
| ATOM | 2589 | CE | LYS A | 325 | 40.358 | 60.464 | 57.850 | 1.00 45.88 | AAAA |
| ATOM | 2590 | NZ | LYS A | 325 | 41.717 | 60.151 | 58.494 | 1.00 46.27 | AAAA |
| | | C | LYS A | | | 59.248 | 56.856 | 1.00 41.56 | AAAA |
| MOTA | 2591 | | | | | | | | |
| MOTA | 2592 | 0 | LYS A | 325 | 35.042 | 58.781 | 55.716 | 1.00 41.35 | AAAA |
| ATOM | 2593 | N | ALA A | 326 | 34.524 | 58.703 | 57.906 | 1.00 41.32 | AAAA |
| | 2594 | CA | ALA A | | 33.732 | 57.492 | 57.774 | 1.00 41.07 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 2595 | CB | ALA A | 326 | 33.452 | 56.912 | 59.143 | 1.00 40.87 | AAAA |
| MOTA | 2596 | С | ALA A | 326 | 32.420 | 57.722 | 57.019 | 1.00 41.24 | AAAA |
| | 2597 | | ALA A | | 32.045 | 56.913 | 56.174 | 1.00 40.91 | AAAA |
| MOTA | | 0 | | | | | | | |
| ATOM | 2598 | N | LYS Y | | 31.719 | 58.815 | 57.316 | 1.00 41.92 | AAAA |
| ATOM | 2599 | CA | LYS A | 327 | 30.451 | 59.097 | 56.631 | 1.00 42.20 | AAAA |
| | 2600 | CB | LYS A | | 29.796 | 60.374 | 57.170 | 1.00 43.61 | AAAA |
| MOTA | | | | | | | | • | |
| MOTA | 2601 | ÇG | LYS A | . 321 | 29.534 | 60.413 | 58,670 | 1.00 45.83 | AAAA |
| ATOM | 2602 | CD | LYS A | . 327 | . 28.745 | 61.681 | 59.029 | 1.00 47.34 | AAAA |
| | 2603 | CE | LYS A | | 28.682 | 61.952 | 60.538 | 1.00 48.28 | AAAA |
| MOTA | | | | | | | | | |
| MOTA | 2604 | NZ | LYS A | | 28.090 | 60.845 | 61.351 | 1.00 48.98 | AAAA |
| ATOM | 2605 | С | LYS A | . 327 | 30.673 | 59.266 | 55.125 | 1.00 41.33 | AAAA |
| ATOM | 2606 | 0 | LYS A | 327 | 29.879 | 58.797 | 54.309 | 1.00 40.78 | AAAA |
| | | | GLU A | | 31,761 | 59.950 | 54.781 | 1.00 40.39 | AAAA |
| ATOM | 2607 | N | | | | | | | |
| ATOM | 2608 | , CA | GLU A | 328 | 32.129 | 60.217 | 53.399 | 1.00 38.91 | AAAA |
| ATOM | 2609 | CB | GLU A | 328 | 33.300 | 61.199 | 53.369 | 1.00 40.04 | AAAA · |
| | 2610 | CG | GLU A | | 32.941 | 62.576 | 53.909 | 1.00 41.94 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2611 | CD | GLU A | | 34.131 | 63.515 | 53.994 | 1.00 43.77 | AAAA |
| ATOM | 2612 | OE1 | GLU A | 328 | 34.904 | 63.595 | 53.010 | 1.00 44.29 | AAAA |
| ATOM | 2613 | OE2 | GLU A | 328 | 34.285 | 64.189 | 55.040 | 1.00 45.11 | AAAA |
| | | | | | 32.497 | | 52.675 | 1.00 37.39 | AAAA |
| MOTA | 2614 | С | GLU A | | | 58.938 | | | |
| ATOM | 2615 | 0 | GLU A | 328 | 32.114 | 58.722 | 51.525 | 1.00 37.31 | AAAA |
| ATOM | 2616 | N | LEU A | 329 | 33.255 | 58.091 | 53.355 | 1.00 35.67 | AAAA |
| | 2617 | CA | LEU A | | 33.657 | 56.820 | 52.783 | 1.00 33.03 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2618 | CB | LEU A | 329 | 34.451 | 56.012 | 53.813 | 1.00 30.62 | AAAA |
| MOTA | 2619 | CG | LEU A | 329 | 34.760 | 54.549 | 53.481 | 1.00 27.48 | AAAA |
| ATOM | 2620 | CD1 | LEU A | 329 | 35.549 | 54.453 | 52.193 | 1.00 36.24 | AAAA |
| | | | | | | | | 1.00 25.74 | AAAA |
| ATOM | 2621 | | LEU A | | 35.514 | 53.936 | 54.622 | | |
| ATOM | 2622 | С | LEU A | 329 | 32.405 | 56.057 | 52.368 | 1.00 33.24 | AAAA |
| ATOM | 2623 | 0 | LEU A | 329 | 32.239 | 55.708 | 51.205 | 1.00 32.72 | AAAA |
| | | N | LEU A | | 31.519 | 55.810 | 53.327 | 1.00 33.92 | AAAA |
| ATOM | 2624 | | | | | | | | |
| MOTA | 2625 | CA | LEU A | | 30.289 | 55.090 | | | AAAA |
| MOTA | 2626 | CB | LEU A | 330 | 29.411 | 55.023 | 54.292 | 1.00 34.02 | AAAA |
| | 2627 | CG | LEU A | | 30.067 | 54.236 | 55.418 | 1.00 34.06 | AAAA |
| ATOM | | | | | | | | 1.00 33.63 | |
| ATOM | . 2628 | | LEU A | | 29.096 | 54.060 | 56.571 | | AAAA |
| ATOM | 2629 | CD2 | LEU A | . 330 | 30.512 | 52.892 | 54.884 | 1.00 33.82 | AAAA |
| ATOM | 2630 | C | LEU A | | 29.499 | 55.695 | 51.907 | 1.00 35.94 | AAAA |
| | | | | | | | 51.060 | 1.00 36.14 | AAAA |
| ATOM | 2631 | 0 | LEU A | | 28.984 | 54.968 | | | |
| MOTA | 2632 | N | LYS A | . 331 | 29.415 | 57.022 | 51.883 | 1.00 38.17 | AAAA |
| ATOM | 2633 | CA | LYS A | 331 | 28,664 | 57.718 | 50.845 | 1.00 41.05 | AAAA |
| | | | LYS A | | | | 51.233 | 1.00 41.83 | AAAA |
| MOTA | 2634 | CB | | | - 28.407 | 59.161 | | | |
| MOTA | 2635 | CG | LYS A | . 331 | 27.584 | 59.358 | 52.497 | 1.00 43.26 | AAAA |
| ATOM | 2636 | CD | LYS A | 331 | 27.202 | 60.823 | 52.755 | 1.00 44.15 | AAAA |
| | | | LYS A | | 26.182 | 61.333 | 51,730 | 1.00 45.71 | AAAA |
| ATOM | 2637 | CE | | | | | | | |
| MOTA | 2638 | NZ | LYS A | | 25.695 | 62.735 | 51.993 | 1.00 45.95 | AAAA |
| MOTA | 2639 | С | LYS A | 331 | 29.342 | 57.681 | 49.490 | 1.00 42.22 | AAAA |
| | 2640 | ŏ | LYS A | | 28.712 | 57.980 | | 1.00 41.94 | AAAA |
| ATOM | 2040 | J | מייים | | 40.114 | 21.300 | | | |
| | | • | | | | | | | |
| | | | | | | | | | |

| ATOM` | 2641 | N. | SER A 332 | | 30.618 | 57.316 | 49,463 | 1.00 44.45 | *** |
|--------|------|-----|-----------|---|--------|--------|--------|------------|--------|
| | | | | | | | | | AAAA |
| MOTA | 2642 | CA | SER A 332 | | 31.351 | 57.271 | 48.202 | 1.00 46.88 | AAAA |
| MOTA | 2643 | CB | SER A 332 | | 32.854 | 57.416 | 48.435 | 1.00 46.49 | AAAA |
| ATOM | 2644 | OG | SER A 332 | | 33.380 | 56.263 | 49.058 | 1.00 45.65 | AAAA |
| ATOM | 2645 | C | SER A 332 | | 31.093 | 55.959 | 47.494 | 1.00 48:73 | AAAA |
| | 2646 | ō | SER A 332 | | 31.262 | 55.854 | 46.281 | | |
| ATOM - | | | | | | | | 1.00 49.51 | AAAA |
| ATOM | 2647 | N | ILE A 333 | | 30.697 | 54.952 | 48.258 | 1.00 50.62 | . AAAA |
| ATOM | 2648 | CA | ILE A 333 | | 30.420 | 53.648 | 47.686 | 1.00 52.65 | AAAA |
| MOTA | 2649 | CB | ILE A.333 | | 30.246 | 52.584 | 48,779 | 1.00 52.35 | AAAA |
| ATOM | 2650 | CG2 | ILE A 333 | | 29.889 | 51.248 | 48.157 | 1.00 51.40 | AAAA |
| ATOM | 2651 | | ILE A 333 | | 31.522 | 52.465 | 49.596 | 1.00 52.29 | AAAA |
| | | | ILE A 333 | | | | | 1.00 52.23 | |
| ATOM | 2652 | | | | 31.403 | 51.463 | | | AAAA |
| MOTA | 2653 | С | ILE A 333 | • | 29.120 | 53.712 | | 1.00 54.42 | AAAA |
| MOTA | 2654 | 0 | ILE A 333 | | 28.122 | 54.178 | 47.462 | 1.00 55.10 | AAAA |
| MOTA | 2655 | N | ASP A 334 | | 29.118 | 53.274 | 45.672 | 1.00 56.56 | AAAA |
| ATOM | 2656 | CA | ASP A 334 | | 27.863 | 53.263 | 44.940 | 1.00 59.13 | - AAAA |
| ATOM | 2657 | CB | ASP A 334 | | 28.050 | 53.460 | 43.433 | 1.00 59.64 | |
| ATOM | 2658 | CG | ASP A 334 | | 28.976 | 52.446 | 42.823 | 1.00 59.23 | AAAA |
| | | | | | | | | | |
| ATOM | 2659 | | ASP A 334 | | 28.853 | 52:194 | 41.606 | 1.00 58.87 | AAAA |
| ATOM | 2660 | | ASP A 334 | | 29.839 | 51.925 | 43.559 | 1.00 59.34 | AAAA |
| MOTA | 2661 | C | ASP A 334 | | 27.251 | 51.898 | 45.215 | 1.00 60.95 | AAAA |
| ATOM | 2662 | Ó | ASP A 334 | | 27.803 | 50.861 | 44.840 | 1.00 61.15 | AAAA |
| MOTA | 2663 | N | PHE A 335 | | 26.113 | 51.914 | 45.897 | 1.00 62.56 | AAAA |
| ATOM | 2664 | CA | PHE A 335 | | 25.414 | 50.701 | 46.257 | 1.00 64.12 | AAAA |
| ATOM . | 2665 | CB | PHE A 335 | | 25.311 | 50.621 | 47.779 | 1.00 64.40 | AAAA |
| | | | | | | 49.714 | 48.263 | | |
| MOTA | 2666 | CG | PHE A 335 | | 24.224 | | | 1.00 64.98 | AAAA |
| MOTA | 2667 | | PHE A 335 | | 24.180 | 48.379 | 47.868 | 1.00 65.54 | AAAA |
| ATOM | 2668 | | PHE A 335 | | 23.234 | 50.197 | 49.107 | 1.00 65.12 | AAAA |
| MOTA | 2669 | CE1 | PHE A 335 | | 23.163 | 47.539 | 48.305 | 1.00 65.75 | AAAA |
| ATOM | 2670 | CE2 | PHE A 335 | | 22.213 | 49.367 | 49.552 | 1.00 65.79 | AAAA |
| ATOM | 2671 | CZ | PHE A 335 | • | 22.177 | 48.034 | 49.150 | 1.00 66.01 | AAAA |
| MOTA | 2672 | C | PHE A 335 | | 24.025 | 50.626 | 45.640 | 1.00 65.41 | AAAA |
| ATOM | 2673 | ŏ | PHE A 335 | | 23.591 | 49.564 | 45.184 | 1.00 65.27 | AAAA |
| | | | | | | | | - | |
| MOTA | 2674 | N | GLU A 336 | | 23.338 | 51.763 | 45.618 | 1.00 66.38 | AAAA |
| MOTA | 2675 | CA | GLU A 336 | | 21.980 | 51.826 | 45.097 | 1.00 67.49 | AAAA |
| MOTA | 2676 | CB | GLU A 336 | | 21.893 | 51.260 | 43.673 | | AAAA |
| ATOM | 2677 | CG | GLU A 336 | | 20.459 | 51.230 | 43.116 | 1.00 69.15 | AAAA |
| ATOM | 2678 | CD | GLU A 336 | | 20.334 | 50.465 | 41.804 | 1.00 69.40 | AAAA |
| ATOM | 2679 | OE1 | GLU A 336 | | 20.710 | 49.271 | 41.784 | 1.00 69.57 | AAAA |
| ATOM | 2680 | | GLU A 336 | | 19.851 | 51.051 | 40.804 | 1.00 69.10 | AAAA |
| ATOM | 2681 | C | GLU A 336 | | 21.098 | 50.999 | 46.025 | 1.00 67.68 | AAAA |
| | | | | | 21.216 | 49.776 | | 1.00 67.58 | AAAA |
| MOTA | 2682 | 0 | GLU A 336 | | | | 46.082 | | |
| ATOM | 2683 | N | GLU A 337 | | 20.227 | 51.679 | 46.761 | 1.00 67.87 | AAAA |
| MOTA | 2684 | CA | GLU A 337 | | 19.317 | 51.020 | 47.686 | 1.00 68.66 | AAAA |
| ATOM | 2685 | CB | GLU A 337 | | 18.583 | 52.085 | 48.502 | 1.00 68.88 | AAAA |
| ATOM | 2686 | CG. | GLU : 337 | | 18.279 | 51.715 | 49.944 | 1.00 68.12 | AAAA |
| ATOM | 2687 | CD | GLU A 337 | | 19.527 | 51.587 | 50.789 | 1.00 67.70 | AAAA |
| ATOM | 2688 | | GLU 337 | | 20.319 | 52.554 | 50.851 | 1.00 67.05 | AAAA |
| | 2689 | | GLU A 337 | | 19.711 | 50.518 | 51.398 | 1.00 67.79 | AAAA |
| ATOM | | | | | 18.322 | | | | |
| MOTA | 2690 | C | GLU A 337 | | | 50.222 | 46.827 | 1.00 69.28 | AAAA |
| ATOM | 2691 | 0 | GLU A 337 | | 17.886 | 50.705 | 45.780 | 1.00 69.50 | AAAA |
| MOTA | 2692 | N | PHE A 338 | | 17.966 | 49.012 | 47.259 | 1.00 69.55 | AAAA |
| MOTA | 2693 | CA | PHE A 338 | | 17.035 | 48.176 | 46.497 | 1.00 69.67 | AAAA |
| MOTA | 2694 | CB | PHE A 338 | | 16.995 | 46.759 | 47.066 | 1.00 70.51 | AAA'A |
| ATOM | 2695 | CG | PHE A 338 | | 16.225 | 45.789 | 46.221 | 1.00 71.57 | AAAA |
| | 2696 | | PHE A 338 | | 16.666 | 45.462 | 44.936 | 1.00 72.04 | AAAA |
| MOTA | | | | | 15.052 | | | 1.00 71.69 | AAAA |
| MOTA | 2697 | | PHE A 338 | | | 45.208 | 46.698 | | |
| MOTA | 2698 | | PHE A 338 | | 15.944 | 44.566 | 44.138 | 1.00 72.23 | AAAA |
| ATOM | 2699 | CE2 | PHE A 338 | | 14.323 | 44.313 | 45.909 | 1.00 71.93 | AAAA |
| MOTA | 2700 | CZ | PHE A 338 | | 14.770 | 43.991 | 44.627 | 1.00 72.11 | AAAA |
| MOTA | 2701 | С | PHE A 338 | | 15.633 | 48.770 | 46.494 | 1.00 69.26 | AAAA |
| ATOM | 2702 | ō | PHE A 338 | | 15.072 | 49.029 | 45.434 | 1.00 68.86 | AAAA |
| | 2703 | N | ASP A 339 | | 15.053 | 48.962 | 47.674 | 1.00 69.35 | AAAA |
| MOTA | | | | | | | | 1.00 69.61 | . AAAA |
| MOTA | 2704 | CA | ASP A 339 | | 13.733 | 49.572 | 47.755 | | |
| ATOM | 2705 | CB | ASP A 339 | | 13.134 | 49.457 | 49.157 | 1.00 69.48 | AAAA |
| MOTA | 2706 | CG | ASP A 339 | | 11.819 | 50.233 | 49.299 | 1.00 69.72 | AAAA |

| 2001 | 2707 | OD1 | ASP A 339 | 11.813 | 51.462 | 49.058 | 1.00 69.39 | AAAA |
|------|--------------|-----|-------------|----------|--------|--------|------------|--------|
| MOTA | 2707 | | ASP A 339 | 10.790 | 49.618 | 49.655 | 1.00 69.78 | AAAA |
| MOTA | | C | ASP A 339 | 13.972 | 51.035 | 47.440 | 1.00 69.95 | AAAA |
| MOTA | 2709 2710 | 0 | ASP A 339 | 14.305 | 51.815 | 48.333 | 1.00 69.92 | AAAA |
| MOTA | - | | ASP A 340 | 13.810 | 51.389 | 46.168 | 1.00 70.23 | AAAA |
| MOTA | 2711 | N | ASP A 340 | 14.023 | 52.748 | 45.699 | 1.00 70.39 | AAAA |
| MOTA | 2712 | CA | | 12.757 | 53.283 | 45.041 | 1.00 70.64 | AAAA |
| ATOM | 2713 | CB | ASP A 340 | 12.737 | 52.517 | 43.791 | 1.00 70.86 | AAAA |
| MOTA | 2714 | CG | ASP A 340 | 12.126 | 51.302 | 43.903 | 1.00 70.93 | AAAA |
| MOTA | 2715 | ODI | ASP A 340 | | 53.125 | 42.699 | 1.00 70.89 | AAAA |
| MOTA | 2716 | | ASP A 340 | 12.399 | 53.674 | 46.807 | 1.00 70.63 | AAAA |
| MOTA | 2717 | С | ASP A 340 | 14.482 | | 47.008 | 1.00 71.13 | AAAA |
| ATOM | 2718 | 0 | ASP A 340 | 15.688 | 53.847 | 47.544 | 1.00 69.95 | AAAA · |
| ATOM | 2719 | N | GLU A 341 | 13.543 | 54.259 | 48.619 | 1.00 69.17 | AAAA |
| ATOM | 2720 | CA | GLU A 341 | 13.947 | 55.150 | 48.266 | 1.00 70.83 | AAAA |
| MOTA | 2721 | CB | GLU A 341 | 13.636 | 56.613 | 49.347 | 1.00 73.44 | AAAA |
| MOTA | 2722 | CG | GLU A 341 | 14.098 | 57.601 | 48.951 | 1.00 75.27 | AAAA |
| ATOM | 2723 | CD | GLU A 341 | 13.956 | 59.071 | | 1.00 76.21 | AAAA |
| ATOM | 2724 | | GLU A 341 | 12.825 | 59.518 | 48.646 | 1.00 75.69 | AAAA |
| ATOM | 2725 | OE2 | GLU A 341 | 14.984 | 59.786 | 48.954 | | AAAA |
| MOTA | 2726 | С | GLU A 341 | 13.367 | 54.819 | 49.983 | 1.00 67.09 | AAAA |
| MOTA | 2727 | 0 | GLU A 341 | 12.233 | 55.176 | 50.297 | 1.00 66.57 | |
| ATOM | 2728 | N | VAL A 342 | . 14.158 | 54.114 | | 1.00 64.87 | AAAA |
| ATOM | 2729 | CA | VAL A 342 | 13.767 | 53.779 | 52.148 | 1.00 62.55 | AAAA |
| ATOM | 2730 | CB | VAL A 342 | 14.265 | 52.377 | 52.589 | 1.00 62.81 | AAAA |
| ATOM | 2731 | | VAL A 342 | 14.042 | 52.193 | 54.081 | 1.00 62.56 | AAAA |
| ATOM | 2732 | CG2 | VAL A 342 | 13.513 | 51.298 | 51.849 | 1.00 63.69 | AAAA |
| ATOM | 2733 | C | VAL A 342 | 14.483 | 54.822 | 52.982 | 1.00 59.94 | AAAA |
| ATOM | 2734 | o | VAL A 342 | 14.022 | 55.215 | 54.054 | 1.00 59.91 | AAAA |
| ATOM | 2735 | N | ASP A 343 | 15.609 | 55.278 | 52.442 | 1.00 56.85 | AAAA |
| MOTA | 2736 | CA | ASP A 343 | 16.457 | 56.266 | 53.085 | 1.00 54.01 | AAAA |
| ATOM | 2737 | СВ | ASP A 343 | 15.639 | 57.446 | 53.605 | 1.00 54.18 | AAAA |
| ATOM | 2738 | CG | ASP A 343 | 16.505 | 58.511 | 54.241 | 1.00 53.96 | AAAA |
| ATOM | 2739 | OD1 | ASP A 343 | 15.947 | 59.485 | 54.785 | 1.00 54.59 | AAAA |
| ATOM | 2740 | OD2 | ASP A 343 | . 17.747 | 58.373 | 54.191 | 1.00 53.61 | AAAA |
| ATOM | 2741 | С | ASP A 343 | 17.186 | 55.609 | 54.242 | 1.00 51.92 | AAAA |
| ATOM | 2742 | 0 | ASP A 343 | 16.611 | 55.371 | 55.307 | 1.00 51.89 | AAAA |
| MOTA | 2743 | N | ARG A 344 | 18.458 | 55.306 | 54.029 | 1.00 48.86 | AAAA |
| ATOM | 2744 | CA | ARG A 344 | 19.240 | 54.676 | 55.069 | 1.00 45.59 | AAAA |
| ATOM | 2745 | CB | ARG A 344 | 19.847 | 53.369 | 54.573 | 1.00 43.94 | AAAA |
| ATOM | 2746 | CG | ARG A 344 | 18.847 | 52.289 | 54.220 | 1.00 41.70 | AAAA |
| ATOM | 2747 | CD | ARG A 344 | 17.953 | 51.955 | 55.385 | 1.00 38.94 | AAAA |
| ATOM | 2748 | NE | ARG A 344 | 17.139 | 50.781 | 55.096 | 1.00 36.78 | AAAA |
| ATOM | 2749 | CZ | ARG A 344 | 16.176 | 50.316 | 55.888 | 1.00 34.81 | . AAAA |
| MOTA | 2750 | NH: | L ARG A 344 | 15.890 | 50.927 | 57.033 | 1.00 34.11 | AAAA |
| MOTA | 2751 | | 2 ARG A 344 | 15.506 | 49.228 | 55.537 | 1.00 31.84 | AAAA. |
| ATOM | 2752 | C | ARG A 344 | 20.340 | 55.604 | 55.520 | 1.00 44.83 | AAAA |
| MOTA | 2753 | ō | ARG A 344 | 21.308 | 55.157 | 56.128 | 1.00 43.97 | AA A |
| ATOM | 2754 | N | SER A 345 | 20.192 | 56.895 | | 1.00 44.32 | A. AA |
| MOTA | 2755 | CA | SER A 345 | 21.199 | 57.877 | | 1.00 43.74 | AAAA |
| ATOM | 2756 | CB | SER A 345 | 20.860 | 59.248 | | 1.00 44.49 | AAAA |
| ATOM | 2757 | OG | SER A 345 | 19.645 | 59.729 | 55.577 | 1.00 46.07 | AAAA |
| | 2758 | c | SER A 345 | 21.307 | 57.977 | 57.144 | 1.00 42.82 | AAAA |
| MOTA | 2759 | | SER A 345 | 22.304 | 58.472 | 57.674 | 1.00 42.91 | AAAA |
| MOTA | 2760 | | TYR A 346 | 20.282 | 57.509 | 57.849 | 1.00 41.48 | AAAA |
| MOTA | 2761 | | TYR A 346 | 20.296 | 57.549 | 59.303 | 1.00 40.35 | AAAA |
| MOTA | 2762 | | TYR A 346 | 18.947 | 57.068 | 59.858 | 1.00 40.38 | . AAAA |
| MOTA | 2763 | | TYR A 346 | 18.630 | | 59.609 | | AAAA |
| MOTA | | | 1 TYR A 346 | 19.293 | 54.589 | | | AAAA |
| MOTA | 2764 | | | 19.022 | | | | AAAA |
| atom | 2765 | | 2 TYR A 346 | 17.682 | | | 1.00 38.49 | AAAA |
| MOTA | 2766 | | | 17.405 | | | 1.00 38.17 | AAAA |
| ATCM | 2767 | | | 18.079 | | | 1.00 37.59 | AAAA |
| ATOM | 2768 | | | | | | 1.00 37.14 | AAAA |
| MOTA | 2769 | | TYR A 346 | 21.436 | | | | AAAA |
| ATOM | 2770 | | LIK W 240 | 21.430 | | | | AAAA |
| MOTA | 2771 | | TYR A 346 | 21.30/ | | | | AAAA |
| MOTE | 2772 | N | MET A 347 | 21.800 | | , | | |

| | 0777 | ~ 3 | MEG | | 242 | 22.879 | 54.756 | 59.530 | 1.00 38.19 | |
|-------|------|-----|-----|---|-------|----------------|--------|--------|-------------|--------|
| MOTA | 2773 | CA | MET | | | | | | | AAAA |
| MOTA | 2774 | CB | MET | Α | 347 | 23.042 | 53.582 | 58.566 | 1.00 38.26 | AAAA |
| MOTA | 2775 | CG | MET | Α | 347 | 21.973 | 52.523 | 58.694 | 1.00 38.17 | AAAA |
| ATOM | 2776 | SD | MET | | | 22.317 | 51.115 | 57.641 | 1.00 38.05 | AAAA |
| | | | | | | | | | • | |
| MOTA | 2777 | CE | MET | | | 22.237 | 51.892 | 56.101 | 1.00 37.61 | AAAA |
| ATOM | 2778 | C | MET | A | 347 | 24.189 | 55.494 | 59.603 | 1.00 38.00 | AAAA |
| MOYA | 2779 | 0 | MET | Α | 347 | 25.127 | 55.033 | 60.250 | 1.00 37.40 | AAAA |
| | | N | | | 348 | 24.248 | 56.637 | 58.929 | 1.00 38.08 | AAAA |
| ATOM | 2780 | | | | | | | | | |
| MOTA | 2781 | CA | LEU | A | 348 | 25.449 | 57.463 | 58.898 | 1.00 38.07 | AAAA |
| MOTA | 2782 | CB | LEU | Α | 348 | 25.445 | 58.330 | 57.638 | 1.00 36.66 | AAAA |
| ATOM | 2783 | CG | LEU | Α | 348 | 25.379 | 57.583 | 56.310 | 1.00 35.47 | AAAA |
| | | | LEU | | | 25.285 | 58.559 | 55.165 | 1.00 34.51 | AAAA |
| MOTA | 2784 | | | | | | | | | |
| ATOM | 2785 | CD2 | LEU | A | 348 | 26.605 | 56.716 | 56.167 | 1.00 36.56 | |
| ATOM- | 2786 | С | LEU | Α | 348 | 25.521 | 58.353 | 60.138 | 1.00 39.07 | AAAA |
| ATOM | 2787 | 0 | LEU | Α | 348 | 26.546 | 58.980 | 60.406 | 1.00 38.81 | AAAA |
| | | И. | | | 349 | 24.432 | 58.385 | 60.898 | 1.00 39.90 | AAAA |
| MOTA | 2788 | | | | | | | | | |
| ATOM | 2789 | CA | GLU | А | 349 | 24.363 | 59,213 | 62.092 | 1.00 40.95 | · AAAA |
| MOTA | 2790 | CB | GLU | Α | 349 | 22.961 | 59.821 | 62.203 | 1.00 41.70 | AAAA |
| MOTA | 2791 | CG | GLU | A | 349 | 22.515 | 60.629 | 60.966 | 1.00 42.28 | AAAA |
| | | | | | | | 61.891 | 60.708 | 1.00 42.51 | AAAA |
| ATOM | 2792 | CD | | | 349 | 23.349 | | | | |
| ATOM | 2793 | | GLU | | | 23.414 | 62,778 | 61.587 | 1.00 42.38 | AAAA |
| MOTA | 2794 | OE2 | GLU | A | 349 | 23.933 | 61.998 | 59.614 | 1.00 43.34 | AAAA |
| | 2795 | C | | | 349 | 24.740 | 58.511 | 63.406 | 1.00 41.12 | AAAA |
| ATOM | | | | | | | | | 1.00 41.38 | AAAA |
| ATOM | 2796 | 0 | | | 349 | 24.664 | 59.118 | 64.476 | | |
| ATOM | 2797 | N | THR | A | 350 | 25.140 | 57.243 | 63.326 | 1.00 40.86 | AAAA |
| ATOM | 2798 | CA | THR | A | 350 | 25.555 | 56.475 | 64.504 | 1.00 40.69 | AAAA |
| ATOM | 2799 | CB | THR | A | 350 | 24.405 | 56.283 | 65.510 | 1.00 41.56 | AAAA |
| | | | | | | 24.062 | 57.549 | 66.078 | 1.00 41.48 | AAAA |
| ATOM | 2800 | | THR | | | | | | | |
| MOTA | 2801 | CG2 | THR | | | 24.821 | 55.345 | 66.638 | 1.00 41.19 | AAAA |
| ATOM | 2802 | С | THR | Α | 350 . | 26.109 | 55.109 | 64.141 | 1.00 40.14 | AAAA |
| MOTA | 2803 | 0 | THR | Α | 350 | 25.857 | 54.595 | 63.055 | 1.00 39.93 | AAAA |
| | | | | | 351 | 26.865 | 54.527 | 65.067 | 1.00 40.32 | AAAA |
| MOTA | 2804 | N | | | | | | | | |
| MOTA | 2805 | CA | LEU | | | 27.491 | 53.227 | 64.857 | 1.00 40.70 | AAAA |
| ATOM | 2806 | CB | LEU | A | 351 | 28.855 | 53.213 | 65.540 | 1.00 39.89 | AAAA |
| ATOM | 2807 | CG | LEU | А | 351 | 29.911 | 52.290 | 64.951 | 1.00 39.68 | AAAA |
| ATOM | 2808 | | LEU | | | 31.170 | 52.403 | 65.772 | 1.00 39.88 | AAAA |
| | | | | | | | | | 1.00 40.70 | AAAA |
| MOTA | 2809 | | LEU | | | 29.414 | 50.861 | 64.945 | | |
| ATOM | 2810 | Ç | LEU | Α | 351 | 26.612 | 52.091 | 65.384 | 1.00 41.12 | AAAA |
| ATOM | 2811 | 0 | LEU | Α | 351 | 26.467 | 51.060 | 64.736 | 1.00 40.02 | AAAA |
| ATOM | 2812 | N | LYS | A | 352 | 26.040 | 52.292 | 66.567 | 1.00 42.99 | AAAA |
| | | | LYS | | | 25.138 | 51.326 | 67.201 | 1.00 43.93 | AAAA |
| MOTA | 2813 | CA | | | | | | | | |
| ATCM | 2814 | CB | LYS | | | 25.412 | 51.225 | 68.707 | 1.00 43.38 | AAAA |
| ATOM | 2815 | CG | LYS | Α | 352 | 26.743 | 50.597 | 69.055 | 1.00 44.68 | AAAA |
| MOTA | 2816 | CD | LYS | Α | 352 | 27.185 | 50.927 | 70.482 | 1.00 45.48 | AAAA |
| | 2817 | CE | LYS | | | 26.189 | 50.500 | 71.539 | 1.00 46.21 | AAAA |
| ATOM | | | | | | | | | 1.00 47.34 | AAAA |
| ATOM | 2818 | NZ | LYS | | | 26.646 | 50.944 | 72.895 | | |
| ATOM | 2819 | С | LYS | | | 23.723 | 51.838 | 67.003 | 1.00 44.40 | AAAA |
| ATOM | 2820 | 0 | LYS | A | 352 | 23.375 | 52.917 | 67.488 | 1.00 45.79 | AAAA |
| ATOM | 2821 | N | ASP | | | 22.904 | 51.083 | 66.287 | 1.00 44.78 | AAAA |
| | | | | | | | 51.509 | 66.074 | 1.00 44.79 | AAAA |
| MOTA | 2822 | CA | ASP | | | 21.532 | | | | |
| MOTA | 2823 | CB | ASP | | | 21.050 | 51.030 | 64.702 | 1.00 45.20 | AAAA |
| ATOM | 2824 | CG | ASP | A | 353 | 21.146 | 49.544 | 64.546 | .1.00 45.21 | AAAA |
| ATOM | 2825 | | ASP | | | 21.806 | 49.086 | 63.581 | 1.00 45.06 | AAAA |
| | | | | | | | | | 1.00 45.54 | AAAA |
| MOTA | 2826 | | ASP | | | 20.549 | 48.841 | 65.391 | | |
| ATOM | 2827 | С | ASP | | | 20.645 | 50.993 | 67.217 | 1.00 44.44 | AAAA |
| ATCM | 2828 | 0 | ASP | | | 21.042 | 50.113 | 67.973 | 1.00 44.29 | AAAA |
| ATOM | 2829 | N | PRO | | | 19.439 | 51.553 | 67.367 | 1.00 44.22 | AAAA |
| | | | | | | | | | 1.00 44.38 | AAAA |
| ATOM | 2830 | CD | PRO | | | 18.839 | 52.617 | 66.550 | | |
| ATCM | 2831 | CA | PRO | Α | 354 | 18.50 0 | 51.163 | 68.419 | 1.00 44.18 | AAAA |
| ATCM | 2832 | CB | PRO | | | 17.371 | 52.170 | 68.238 | 1.00 44.52 | AAAA |
| | | | PRO | | | 17.368 | 52.341 | 66.749 | 1.00 44.66 | AAAA |
| ATCM | 2833 | CG | | | | | | | 1.00 43.87 | AAAA |
| ATCM | 2834 | С | PRO | A | 334 | 17.995 | 49.740 | 68.328 | | |
| ATCM. | 2835 | 0 | PRO | Α | 354 | 17.962 | 49.152 | 67.249 | 1.00 44.48 | AAAA |
| ATCM | 2836 | N | TRP | | | 17.588 | 49.198 | 69.469 | 1.00 43.23 | AAAA |
| | _ | | TRP | | | 17.051 | 47.851 | 69.500 | 1.00 42.88 | AAAA |
| ATOM | 2837 | CA | | | | | | | 1.00 46.42 | AAAA. |
| ATCM | 2838 | CB | TRP | A | 222 | 16.743 | 47.401 | 70.927 | 1.00 40.42 | |
| | | | - | | | | | - | | • |

| 3 mov | 2020 | ~~ | mn | 255 | 17 050 | 47 050 | 71 606 | 1 00 40 01 | |
|--------|------|-----|-------|-------|--------|--------|--------|------------|--------|
| ATOM | 2839 | CG | TRP A | | 17.959 | 47.052 | 71.695 | 1.00 49.91 | AAAA |
| ATOM | 2840 | CD2 | TRP A | 355 | 18.476 | 45.733 | 71.903 | 1.00 51.56 | AAAA |
| ATOM | 2841 | CE2 | TRP A | 355 | 19.684 | 45.868 | 72.627 | 1.00 52.03 | AAAA |
| | | | TRP A | | | | | | |
| MOTA | 2842 | CE3 | | | 18.038 | 44.450 | 71.548 | 1.00 52.25 | AAAA |
| ATOM | 2843 | CD1 | TRP A | 355 | 18.846 | 47.915 | 72.284 | 1.00 50.53 | AAAA |
| ATOM | 2844 | NE1 | TRP A | 355 | 19.885 | 47208 | 72.846 | 1.00 51.63 | AAAA |
| | 2845 | CZ2 | TRP A | | 20.460 | 44.763 | 73.003 | 1.00 52.64 | AAAA |
| MOTA | • | | _ | | | | | | |
| ATOM . | 2846 | CZ3 | TRP A | 355 | 18.810 | 43.352 | 71.921 | 1.00 53.12 | AAAA |
| ATOM | 2847 | CH2 | TRP A | 355 | 20.008 | 43:518 | 72.642 | 1.00 53.02 | AAAA |
| | | C | TRP A | | 15.788 | 47.767 | 68.675 | 1.00 40.28 | AAAA |
| ATOM | 2848 | | | | | | | | |
| MOTA | 2849 | 0 | TRP A | 355 | 15.017 | 48.720 | 68.591 | 1.00 39.82 | AAAA |
| ATOM | 2850 | N | ARG A | 356 | 15.591 | 46.610 | 68.065 | 1.00 36.83 | AAAA |
| ATOM | 2851 | CA | ARG A | | 14.440 | 46.365 | 67.225 | 1.00 33.70 | ÄAAA |
| | _ | | | | | | | | |
| MOTA | 2852 | СВ | ARG A | | 14.901 | 46.197 | 65.772 | 1.00 29.50 | AAAA |
| ATOM | 2853 | CG | ARG A | 356 | 15.635 | 47.423 | 65.256 | 1.00 25.22 | AAAA |
| ATOM | 2854 | CD | ARG A | 356 | 16.418 | 47.194 | 63.973 | 1.00 21.53 | AAAA |
| | | | | | 17.055 | 48.435 | 63.533 | 1.00 18.55 | AAAA |
| MOTA | 2855 | NE | ARG A | | | | | | |
| MOTA | 2856 | CZ | ARG A | 356 | 17.976 | 48.533 | 62.574 | 1.00 17.06 | AAAA |
| ATOM | 2857 | NH1 | ARG A | 356 | 18.403 | 47.451 | 61.919 | 1.00 17.64 | AAAA |
| | 2858 | NH2 | ARG A | | 18.445 | 49.721 | 62.241 | 1.00 11.56 | AAAA |
| MOTA | | | | | | | | | |
| MOTA | 2859 | С | ARG A | | 13.831 | 45.095 | 67.773 | 1.00 34.63 | AAAA |
| ATOM | 2860 | 0 | ARG A | 356 | 13.605 | 44.117 | 67.051 | 1.00 35.86 | AAAA |
| ATOM | 2861 | N | GLY A | 357 | 13.587 | 45.112 | 69.079 | 1.00 34.58 | AAAA |
| | | - | GLY A | | 13.003 | 43.960 | 69.734 | 1.00 34.33 | AAAA |
| ATOM | 2862 | CA | | | | | | | |
| ATOM | 2863 | С | GLY A | | 11.536 | 43.783 | 69.395 | 1.00 34.31 | AAAA |
| ATOM | 2864 | 0 | GLY A | 357 | 11.006 | 44.418 | 68.484 | 1.00 33.56 | AAAA |
| MOTA | 2865 | N | GLY A | 358 | 10.876 | 42.906 | 70.139 | 1.00 34.47 | AAAA |
| | | CA | GLY A | | 9.468 | 42.656 | 69.916 | 1.00 34.61 | AAAA |
| MOTA | 2866 | | | | | | | | |
| MOTA | 2867 | С | GĻY A | | 9.114 | 41.389 | 70.655 | 1.00 34.47 | , AAAA |
| ATOM- | 2868 | 0 | GLY A | 358 | 9.962 | 40.821 | 71.345 | 1.00 34.27 | AAAA |
| ATOM | 2869 | N | GLU A | 359 | 7.869 | 40.948 | 70.523 | 1.00 34.16 | AAAA |
| | | CA | GLU A | | 7.438 | 39.729 | 71.180 | 1.00 33.94 | AAAA |
| ATOM | 2870 | | | | | | | | |
| ATOM | 2871 | CB | GLU A | | 5.910 | 39.644 | 71.174 | 1.00 34.78 | AAAA |
| MOTA | 2872 | ÇG | GLU A | 359 | 5.278 | 40.648 | 72.123 | 1.00 36.70 | AAAA |
| MOTA | 2873 | ĊD | GLU A | 359 | 3.863 | 41.020 | 71.740 | 1.00 38.40 | AAAA |
| | 2874 | | GLU A | | 3.017 | 40.108 | 71.600 | 1.00 39.65 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 2875 | | GLU A | | 3.598 | 42.234 | 71.584 | 1.00 38.52 | AAAA |
| ATOM | 2876 | С | GLU A | 359 | 8.058 | 38.549 | 70.464 | 1.00 32.86 | AAAA |
| ATOM | 2877 | 0 | GLU A | 359 | 8.678 | 38.692 | 69.427 | 1.00 32.92 | AAAA |
| | 2878 | N | VAL A | | 7.918 | 37.375 | 71.036 | 1.00 32.63 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2879 | CA | VAL A | | 8.480 | 36.215 | 70.409 | 1.00 32.70 | AAAA |
| ATOM | 2880 | CB | VAL A | 1 360 | 9.422 | 35.472 | 71.376 | 1.00 33.24 | AAAA |
| ATOM | 2881 | CG1 | VAL A | 360 | 10.017 | 34.252 | 70.701 | 1.00 32.99 | AAAA |
| | 2882 | | VAL A | | 10.521 | 36.406 | 71.827 | 1.00 32.09 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2883 | С | VAL A | | 7.339 | 35.319 | 69.976 | 1.00 32.81 | AAAA |
| MOTA | 2884 | 0 | VAL A | 360 | 6.702 | 34.660 | 70.791 | 1.00 32.02 | AAAA |
| ATOM | 2885 | N | ARG A | 361 | 7.084 | 35.321 | 68.674 | 1.00 33.12 | AAAA |
| | 2886 | CA | ARG A | | 6.035 | 34.508 | 68.086 | 1.00 33.52 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 2887 | CB | ARG A | | 6.148 | 34.558 | 66.565 | 1.00 33.43 | AAAA |
| MOTA | 2888 | CG | ARG A | 361 | 5.731 | 35.885 | 65.967 | 1.00 34.35 | AAAA |
| ATOM | 2889 | CD | ARG A | 361 | 6.041 | 35.972 | 64.469 | 1.00 33.90 | AAAA |
| | 2890 | NE | ARG A | | 7.430 | 36.331 | 64.193 | 1.00 31.70 | AAAA |
| ATOM | | | | | | | | 1.00 31.18 | AAAA |
| ATOM | 2891 | CZ | ARG A | | 7.890 | 36.608 | 62.978 | | |
| ATOM | 2892 | NH1 | ARG A | 361 | 7.068 | 36.562 | 61.941 | 1.00 30.48 | AAAA |
| MOTA | 2893 | NH2 | ARG A | 361 | 9.162 | 36.948 | 62.802 | 1.00 29.71 | AAAA |
| | 2894 | C | ARG A | | 6.066 | 33.057 | 68.557 | 1.00 34.20 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2895 | 0 | ARG A | | 7.101 | 32.537 | 68.968 | 1.00 33.79 | AAAA |
| ATOM | 2896 | N | LYS A | 362 | 4.914 | 32.407 | 68.496 | 1.00 34.68 | AAAA |
| ATOM | 2897 | CA | LYS A | | 4.808 | 31.022 | 68.901 | 1.00 35.62 | AAAA |
| | | CB | LYS A | | 3.350 | 30.555 | 68.782 | 1.00 37.80 | AAAA |
| ATOM | 2898 | | | | | | | | |
| ATOM | 2899 | CG | LYS ? | | 2.378 | 31.226 | 69.756 | 1.00 40.38 | AAAA |
| MOTA | 2900 | CD | LYS A | | 2.505 | 32.777 | 69.777 | 1.00 42.09 | AAAA |
| ATOM | 2901 | CE | LYS A | | 2.208 | 33.446 | 68.420 | 1.00 41.94 | AAAA |
| | | NZ | LYS A | | 2.473 | 34.909 | 68.451 | 1.00 39.85 | AAAA |
| ATOM | 2902 | | | | | | | | |
| ATCM | 2903 | С | LYS A | | 5.710 | 30.177 | 68.005 | 1.00 35.12 | AAAA |
| ATOM | 2904 | Ο. | LYS A | A 362 | 6.425 | 29.301 | 68.487 | 1.00 34.14 | AAAA |
| | - | - | | | | | - | | |

| ATOM 2916 CA CLU À 363 6.445 29.741 65.699 1.00 35.62 AAAA ATOM 2910 CB CLU À 363 5.280 30.808 63.711 1.00 38.66 AAAA ATOM 2910 CB CLU À 363 5.280 30.808 63.711 1.00 38.66 AAAA ATOM 2910 CB CLU À 363 5.280 30.808 63.711 1.00 38.66 AAAA ATOM 2911 CBC CLU À 363 6.287 31.324 61.637 1.00 39.10 AAAA ATOM 2911 CBC CLU À 363 6.287 31.324 61.637 1.00 39.11 AAAA ATOM 2912 C CLU À 363 4.826 32.782 62.469 1.00 39.95 AAAA ATOM 2912 C CLU À 363 4.826 32.782 62.469 1.00 39.95 AAAA ATOM 2912 C CLU À 363 4.826 32.782 62.469 1.00 39.95 AAAA ATOM 2912 C CLU À 363 4.826 32.782 62.469 1.00 39.95 AAAA ATOM 2912 C CLU À 363 4.826 32.782 62.469 1.00 39.95 AAAA ATOM 2914 N VAL À 364 8.475 30.505 66.671 1.00 34.96 AAAA ATOM 2915 CA VAL À 364 8.475 30.505 66.671 1.00 34.96 AAAA ATOM 2915 CA VAL À 364 10.338 31.821 67.570 1.00 33.68 AAAA ATOM 2915 C VAL À 364 10.338 31.821 67.570 1.00 33.68 AAAA ATOM 2918 C VAL À 364 10.337 32.715 66.347 1.00 33.48 AAAA ATOM 2919 C VAL À 364 10.337 32.715 66.347 1.00 31.83 AAAA ATOM 2919 C VAL À 364 10.337 32.715 66.347 1.00 31.83 AAAA ATOM 2921 N LYS À 365 8.890 28.690 68.430 1.00 33.61 AAAA ATOM 2921 C VAL À 364 10.789 28.640 68.430 1.00 36.01 AAAA ATOM 2922 CA LYS À 365 8.890 28.690 68.430 1.00 33.20 AAAA ATOM 2922 CA LYS À 365 8.890 28.690 68.430 1.00 33.20 AAAA ATOM 2922 C CL LYS À 365 8.890 28.690 68.430 1.00 33.20 AAAA ATOM 2922 C CL LYS À 365 8.890 28.390 70.476 1.00 33.20 AAAA ATOM 2922 C CL LYS À 365 8.890 28.390 70.476 1.00 33.20 AAAA ATOM 2924 C CL LYS À 365 8.890 28.390 70.476 1.00 33.20 AAAA ATOM 2925 C CL LYS À 365 8.890 28.390 70.476 1.00 33.20 AAAA ATOM 2925 C CL LYS À 365 8.890 28.390 70.476 1.00 33.20 AAAA ATOM 2926 C CL LYS À 365 8.890 28.390 70.476 1.00 33.20 AAAA ATOM 2927 C CL LYS À 365 8.890 28.390 70.476 1.00 33.20 AAAA ATOM 2928 C CL LYS À 365 8.890 28.390 28.390 70.476 1.00 33.20 AAAA ATOM 2929 C CL LYS À 365 8.890 28.390 28.390 70.476 1.00 33.20 AAAA ATOM 2929 C CL LYS À 366 8.890 28.390 28.390 70.476 1.00 33.69 AAAA ATOM 2929 C CL LYS À 366 8.890 28.390 28.390 28.390 1.00 33. | 3000 | 2905 | N . | GLU A | 363 | 5,661 | 30.460 | 66.703 | 1.00 35.12 | AAAA |
|--|--------|------|-----|-------|-------|--------|--------|--------|------------|-----------|
| ATOM 2907 CE GLU A 363 6.567 30.560 64.424 1.00 36.81 AAAA ATOM 2908 CG GLU A 363 5.280 30.808 63.711 1.00 38.66 AAAA ATOM 2910 OEI GLU A 363 5.280 30.808 63.711 1.00 38.66 AAAA ATOM 2911 OEI GLU A 363 6.287 31.324 61.637 1.00 39.11 AAAA ATOM 2911 OEI GLU A 363 4.826 32.782 62.469 1.00 39.11 AAAA ATOM 2912 C GLU A 363 4.826 32.782 62.469 1.00 39.91 AAAA ATOM 2913 O GLU A 363 8.321 28.316 66.098 1.00 34.50 AAAA ATOM 2913 N VAL A 364 8.475 30.505 66.671 1.00 34.50 AAAA ATOM 2915 CA VAL A 364 9.830 30.431 67.180 1.00 34.96 AAAA ATOM 2915 CC VAL A 364 9.830 30.431 67.180 1.00 34.44 AAAA ATOM 2915 CC VAL A 364 10.338 31.821 67.570 1.00 34.44 AAAA ATOM 2919 C CV AL A 364 10.338 31.821 67.570 1.00 34.13 AAAA ATOM 2919 C CV AL A 364 10.337 31.722 68.162 1.00 34.13 AAAA ATOM 2919 C CV AL A 364 9.908 29.499 68.370 1.00 34.44 AAAA ATOM 2920 C VAL A 364 9.908 29.499 68.370 1.00 34.44 AAAA ATOM 2921 N LYS A 365 8.990 29.649 69.305 1.00 33.68 AAAA ATOM 2922 CA LYS A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CL LYS A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CL LYS A 365 7.282 311.181 73.039 1.00 34.83 AAAA ATOM 2925 CC LYS A 365 7.282 311.181 73.039 1.00 34.83 AAAA ATOM 2925 CL LYS A 365 7.282 311.811 73.039 1.00 34.83 AAAA ATOM 2925 CL LYS A 365 7.282 311.811 73.039 1.00 34.83 AAAA ATOM 2927 NZ LYS A 365 8.890 29.649 69.305 1.00 33.27 AAAA ATOM 2928 C LYS A 365 7.282 311.181 73.039 1.00 34.83 AAAA ATOM 2929 C LYS A 365 7.282 311.181 73.039 1.00 34.85 AAAA ATOM 2929 C LYS A 365 7.282 311.181 73.039 1.00 34.85 AAAA ATOM 2929 C LYS A 365 8.8970 28.797 70.7476 1.00 33.267 AAAA ATOM 2929 C LYS A 365 8.8970 28.797 70.476 1.00 33.275 AAAA ATOM 2929 C LYS A 365 8.8970 28.797 70.00 33.00 33.67 AAAA ATOM 2929 C LYS A 365 8.8970 28.797 70.00 33.00 33.67 AAAA ATOM 2929 C LYS A 365 8.8970 28.797 70.00 33.00 33.67 AAAA ATOM 2929 C LYS A 365 8.8970 28.797 70.00 33.00 33.67 AAAA ATOM 2929 C LYS A 365 8.8970 28.797 70.00 33.00 33.67 AAAA ATOM 2929 C LYS A 365 8.8970 | | | | | | | | | | |
| ATOM 2908 CG GLU A 363 5.280 30.808 63.711 1.00 38.66 AAAA ATOM 2910 CD GLU A 363 6.287 31.324 61.637 1.00 39.60 AAAA ATOM 2911 OSE GLU A 363 6.287 31.324 61.637 1.00 39.11 AAAA ATOM 2912 CC GLU A 363 7.836 29.450 66.181 1.00 35.14 AAAA ATOM 2913 OSE GLU A 363 7.836 29.450 66.181 1.00 35.14 AAAA ATOM 2915 CA VAL A 364 8.475 30.505 66.671 1.00 34.50 AAAA ATOM 2915 CA VAL A 364 8.475 30.505 66.671 1.00 34.50 AAAA ATOM 2915 CA VAL A 364 8.475 30.505 66.671 1.00 34.44 AAAA ATOM 2915 CA VAL A 364 10.338 31.821 67.570 1.00 33.68 AAAA ATOM 2915 CA VAL A 364 10.338 31.821 67.570 1.00 33.68 AAAA ATOM 2915 CA VAL A 364 10.337 32.715 66.347 1.00 34.44 AAAA ATOM 2915 CC VAL A 364 10.337 32.715 66.347 1.00 31.68 AAAA ATOM 2919 C VAL A 364 10.337 32.715 66.347 1.00 31.68 AAAA ATOM 2919 C VAL A 364 10.337 32.715 66.347 1.00 31.63 AAAA ATOM 2920 O VAL A 364 10.739 28.640 68.430 1.00 36.01 AAAA ATOM 2921 N LYS A 365 8.980 29.499 68.370 1.00 33.27 AAAA ATOM 2921 N LYS A 365 8.980 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.980 29.649 69.305 1.00 33.20 AAAA ATOM 2922 CB LYS A 365 7.968 29.319 71.508 1.00 33.20 AAAA ATOM 2922 CB LYS A 365 7.968 29.319 71.508 1.00 33.428 AAAA ATOM 2922 CB LYS A 365 7.968 32.534 73.638 1.00 34.43 AAAA ATOM 2929 CC LYS A 365 7.698 32.534 73.638 1.00 34.43 AAAA ATOM 2929 CC LYS A 365 7.698 32.534 73.638 1.00 34.43 AAAA ATOM 2929 CC LYS A 365 7.698 32.534 73.638 1.00 34.43 AAAA ATOM 2929 CC LYS A 365 7.698 32.534 73.638 1.00 33.47 AAAA ATOM 2928 C LYS A 365 7.602 5.777 68.501 30.30 1.00 33.47 AAAA ATOM 2928 C LYS A 365 7.602 5.777 68.60 30.30 1.00 33.48 AAAA ATOM 2930 N ASP A 366 6.698 25.797 69.012 1.00 32.75 AAAA ATOM 2931 CA ASP A 366 7.909 27.136 69.012 1.00 32.75 AAAA ATOM 2934 OD ASP A 366 6.699 25.777 69.501 1.00 33.98 AAAA ATOM 2934 OD ASP A 366 6.599 25.776 69.307 1.00 33.98 AAAA ATOM 2934 OD ASP A 366 6.599 25.776 69.307 1.00 33.68 AAAA ATOM 2935 CD ASP A 366 6.599 25.776 69.307 1.00 33.68 AAAA ATOM 2936 C ASP A 366 6.599 25.776 69.307 1.00 33.68 AAAA ATOM 2936 C ASP A 366 6.599 25 | | | | | | | | | | |
| ATOM 2909 CD GLU A 363 5.477 31.704 62.517 1.00 39.60 AAAA ATOM 2911 OSI GLU A 363 6.287 31.324 61.637 1.00 39.11 AAAA ATOM 2912 C GLU A 363 4.826 32.782 62.469 1.00 39.15 AAAA ATOM 2913 OSI GLU A 363 4.826 32.782 62.469 1.00 39.15 AAAA ATOM 2913 OSI GLU A 363 8.321 28.316 66.098 1.00 34.50 AAAA ATOM 2914 N VAL A 364 8.475 30.505 66.671 1.00 34.50 AAAA ATOM 2915 CA VAL A 364 9.830 30.431 67.180 1.00 34.96 AAAA ATOM 2915 CB VAL A 364 9.830 30.431 67.180 1.00 34.44 AAAA ATOM 2915 CB VAL A 364 10.338 31.821 67.570 1.00 34.44 AAAA ATOM 2916 CB VAL A 364 10.338 31.821 67.570 1.00 34.44 AAAA ATOM 2919 C CV AL A 364 10.337 31.722 68.162 1.00 34.13 AAAA ATOM 2919 C CV AL A 364 10.337 31.722 68.162 1.00 34.13 AAAA ATOM 2920 C VAL A 364 9.908 29.499 68.370 1.00 34.44 AAAA ATOM 2920 C VAL A 364 9.908 29.499 68.370 1.00 34.44 AAAA ATOM 2921 N LYS A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CL LYS A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2925 CD LYS A 365 7.282 31.181 73.039 1.00 34.83 AAAA ATOM 2925 CD LYS A 365 7.282 31.181 73.039 1.00 34.85 AAAA ATOM 2925 CD LYS A 365 7.282 31.181 73.039 1.00 34.85 AAAA ATOM 2926 CE LYS A 365 7.282 31.181 73.039 1.00 34.85 AAAA ATOM 2927 NZ LYS A 365 8.594 72.82 31.181 73.039 1.00 34.85 AAAA ATOM 2927 CD LYS A 365 6.698 32.990 74.710 1.00 37.91 AAAA ATOM 2928 C LYS A 365 6.698 32.990 74.710 1.00 37.91 AAAA ATOM 2929 C LYS A 365 8.544 77.342 70.109 1.00 33.647 AAAA ATOM 2929 C LYS A 365 8.544 77.342 70.109 1.00 33.64 7 AAAA ATOM 2921 CD LYS A 365 8.544 77.342 70.109 1.00 33.86 AAAA ATOM 2931 CA ASP A 366 6.542 70.000 25.777 68.511 1.00 33.94 AAAA ATOM 2931 CA ASP A 366 6.542 70.000 25.777 68.511 1.00 33.94 AAAA ATOM 2931 CA ASP A 366 6.542 70.000 25.777 68.511 1.00 33.93 AAAA ATOM 2931 CA ASP A 366 8.511 1.000 25.777 69.511 1.00 33.93 AAAA ATOM 2931 CA ASP A 366 8.511 1.000 25.777 69.501 1.000 33.94 AAAA ATOM 2931 CA ASP A 366 8.511 1.000 25.777 69.501 1.000 | | | | | | | - | | | |
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| ATOM 2911 OEZ GLU A 363 4.826 32.782 62.469 1.00 39.95 AAAA ATOM 2912 C GLU A 363 8.321 28.316 66.098 1.00 35.14 AAAA ATOM 2913 O GLU A 363 8.321 28.316 66.098 1.00 34.50 AAAA ATOM 2915 CA VAL A 364 9.830 30.431 67.180 1.00 34.96 AAAA ATOM 2915 CB VAL A 364 9.830 30.431 67.180 1.00 34.96 AAAA ATOM 2915 CB VAL A 364 10.338 31.821 67.570 1.00 34.44 AAAA ATOM 2917 CGI VAL A 364 11.739 31.722 68.162 1.00 34.13 AAAA ATOM 2919 C CZ VAL A 364 11.739 31.722 68.162 1.00 34.13 AAAA ATOM 2919 C CZ VAL A 364 11.739 31.722 68.162 1.00 34.13 AAAA ATOM 2919 C CZ VAL A 364 10.337 31.821 67.570 1.00 34.14 AAAA ATOM 2919 C VAL A 364 9.908 29.499 68.370 1.00 34.44 AAAA ATOM 2919 C VAL A 364 9.908 29.499 68.370 1.00 34.44 AAAA ATOM 2921 N LY5 A 365 8.990 29.649 68.430 1.00 35.01 AAAA ATOM 2922 C LY5 A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 C LY5 A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 C LY5 A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 C LY5 A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 C LY5 A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 C LY5 A 365 8.990 29.549 69.305 1.00 33.27 AAAA ATOM 2922 C LY5 A 365 7.968 29.319 71.508 1.00 34.85 AAAA ATOM 2922 C LY5 A 365 7.968 29.319 71.508 1.00 34.85 AAAA ATOM 2925 CD LY5 A 365 7.658 3.207 30.705 72.033 1.00 34.65 AAAA ATOM 2925 CD LY5 A 365 7.658 32.534 73.638 1.00 33.67 AAAA ATOM 2925 CD LY5 A 365 6.698 32.990 74.710 1.00 37.91 AAAA ATOM 2926 CE LY5 A 365 8.654 7.912 7.710 0.00 37.91 AAAA ATOM 2927 NZ LY5 A 365 8.654 7.912 7.7136 69.012 1.00 33.98 AAAA ATOM 2929 C LY5 A 365 8.654 7.912 7.7136 69.012 1.00 33.98 AAAA ATOM 2933 C B ASP A 366 7.919 27.136 69.012 1.00 33.95 AAAA ATOM 2933 C B ASP A 366 7.919 27.136 69.012 1.00 33.98 AAAA ATOM 2935 C SAP A 366 5.459 25.767 69.307 1.00 31.05 3.98 AAAA ATOM 2935 C SAP A 366 5.459 25.766 69.307 1.00 30.05 3.89 AAAA ATOM 2935 C SAP A 366 6.459 25.767 69.001 1.00 30.93 AAAA ATOM 2935 C C LYS A 365 8.654 7.919 27.136 69.012 1.00 33.98 AAAA ATOM 2935 C C LYS A 366 7.910 1.00 30.05 AAAA ATOM 2935 C C LYS A 36 | | - | | | | | | | | |
| ATOM 2912 C GLU A 363 7.836 29.450 66.181 1.00 35.14 AAAA ATOM 2913 0 GLU A 363 8.321 28.316 66.098 1.00 34.50 AAAA ATOM 2915 CA VAL A 364 8.475 30.505 66.671 1.00 34.96 AAAA ATOM 2915 CA VAL A 364 10.338 31.821 67.570 1.00 33.68 AAAA ATOM 2915 CA VAL A 364 10.338 31.821 67.570 1.00 33.68 AAAA ATOM 2917 CG1 VAL A 364 10.338 31.821 67.570 1.00 33.68 AAAA ATOM 2917 CG1 VAL A 364 11.739 31.722 68.162 1.00 34.13 AAAA ATOM 2918 CG2 VAL A 364 10.337 32.715 66.347 1.00 31.83 AAAA ATOM 2918 CG2 VAL A 364 10.337 32.715 66.347 1.00 31.83 AAAA ATOM 2918 CG2 VAL A 364 10.337 32.715 66.347 1.00 31.83 AAAA ATOM 2919 C VAL A 364 10.739 28.499 68.370 1.00 31.44 AAAA ATOM 2921 N LYS A 365 8.980 29.499 68.370 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.980 29.499 68.370 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.980 29.499 68.370 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.980 29.399 70.476 1.00 33.27 AAAA ATOM 2922 CG LYS A 365 7.988 29.319 71.508 1.00 34.28 AAAA ATOM 2925 CD LYS A 365 7.282 31.715 81.00 34.28 AAAA ATOM 2925 CD LYS A 365 7.282 31.715 81.00 34.28 AAAA ATOM 2925 CC LYS A 365 7.282 31.715 81.00 34.85 AAAA ATOM 2926 CE LYS A 365 7.282 31.715 81.00 34.85 AAAA ATOM 2926 CE LYS A 365 8.584 77.588 32.534 73.039 1.00 34.67 91.40 AAAA ATOM 2927 NZ LYS A 365 8.654 27.342 70.109 1.00 32.75 AAAA ATOM 2921 C LYS A 365 8.654 27.342 70.10 1.00 32.75 AAAA ATOM 2921 C LYS A 365 8.654 27.342 70.10 1.00 32.75 AAAA ATOM 2931 CA ASP A 366 7.600 25.777 68.581 1.00 31.95 AAAA ATOM 2931 CA ASP A 366 7.600 25.777 68.581 1.00 32.95 AAAA ATOM 2932 C LYS A 365 8.654 27.342 70.10 1.00 32.75 AAAA ATOM 2931 CA ASP A 366 7.500 25.777 68.581 1.00 32.95 AAAA ATOM 2931 CA ASP A 366 5.131 26.10 0.00 22.75 AAAA ATOM 2931 CA ASP A 366 5.131 26.10 0.00 22.75 AAAA ATOM 2935 C ASP A 366 5.131 26.10 0.00 22.75 AAAA ATOM 2935 C ASP A 366 5.131 26.10 0.00 22.75 AAAA ATOM 2935 C ASP A 366 5.131 26.10 0.00 22.75 AAAA ATOM 2935 C ASP A 366 5.131 26.10 0.00 22.75 AAAA ATOM 2935 C ASP A 366 5.131 26.25 AAAA ATOM 2935 C ASP A 366 5.131 26.25 AAAA ATOM 2935 C ASP A 366 | | - | | | | | | | | |
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| ATOM 2916 CB VAL A 364 9.830 30.431 67.180 1.00 34.44 AAAA ATOM 2917 CG1 VAL A 364 10.338 31.821 67.570 1.00 33.68 AAAA ATOM 2919 C VAL A 364 10.337 31.722 68.162 1.00 34.13 AAAA ATOM 2919 C VAL A 364 9.908 29.499 68.370 1.00 34.44 AAAA ATOM 2919 C VAL A 364 9.908 29.499 68.370 1.00 34.44 AAAA ATOM 2920 O VAL A 364 9.908 29.499 68.370 1.00 34.44 AAAA ATOM 2921 N LYS A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.990 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.990 29.319 71.508 1.00 34.28 AAAA ATOM 2924 CG LYS A 365 7.968 29.319 71.508 1.00 34.28 AAAA ATOM 2925 CD LYS A 365 7.282 31.181 73.039 1.00 34.85 AAAA ATOM 2926 CE LYS A 365 7.282 31.181 73.039 1.00 34.87 AAAA ATOM 2927 72 LYS A 365 6.698 32.590 74.710 1.00 37.91 AAAA ATOM 2928 C LYS A 365 8.654 27.342 70.109 1.00 32.75 AAAA ATOM 2929 O LYS A 365 8.654 27.342 70.109 1.00 32.75 AAAA ATOM 2929 O LYS A 365 8.654 27.342 70.109 1.00 32.75 AAAA ATOM 2930 N ASP A 366 7.600 25.777 68.821 70.618 1.00 34.85 AAAA ATOM 2931 CA ASP A 366 7.600 25.777 68.811 70.00 31.95 AAAA ATOM 2932 CB ASP A 366 7.600 25.777 68.811 70.00 31.95 AAAA ATOM 2933 CA ASP A 366 6.459 25.726 67.557 1.00 31.98 AAAA ATOM 2934 ODI ASP A 366 6.459 25.776 68.381 1.00 34.85 AAAA ATOM 2935 OZ ASP A 366 6.459 25.777 68.811 1.00 31.98 AAAA ATOM 2936 C ASP A 366 6.459 25.777 68.141 1.00 31.98 AAAA ATOM 2936 C ASP A 366 6.459 25.777 68.141 1.00 31.98 AAAA ATOM 2936 C ASP A 366 6.459 25.777 68.141 1.00 31.98 AAAA ATOM 2936 C AS | • | | | - | | | | | | |
| ATOM 2916 CB VAL A 364 10.338 31.821 67.570 1.00 33.68 AAAA ATOM 2918 CG2 VAL A 364 10.739 31.722 68.162 -1.00 34.13 AAAA ATOM 2918 CG2 VAL A 364 10.337 32.715 66.347 1.00 31.83 AAAA ATOM 2919 C VAL A 364 10.789 28.640 68.430 1.00 36.01 AAAA ATOM 2920 O VAL A 364 10.789 28.640 68.430 1.00 36.01 AAAA ATOM 2921 N LYS A 365 8.980 29.499 68.370 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.980 29.499 69.505 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.980 29.499 70.476 1.00 33.20 AAAA ATOM 2923 CG LYS A 365 7.568 29.319 71.067 10.03 32.20 AAAA ATOM 2925 CD LYS A 365 7.568 29.319 71.00 31.00 34.28 AAAA ATOM 2925 CD LYS A 365 7.282 31.181 73.039 1.00 34.85 AAAA ATOM 2925 CD LYS A 365 7.658 29.319 71.00 34.85 AAAA ATOM 2927 NZ LYS A 365 6.698 32.990 74.710 1.00 37.91 AAAA ATOM 2929 C LYS A 365 6.698 32.990 74.710 1.00 37.91 AAAA ATOM 2929 C LYS A 365 8.567 7.658 32.534 70.109 1.00 32.75 AAAA ATOM 2929 C LYS A 365 9.071 26.421 70.818 1.00 31.95 AAAA ATOM 2929 C LYS A 3665 9.071 26.421 70.818 1.00 31.95 AAAA ATOM 2929 C LYS A 3665 9.071 26.421 70.818 1.00 31.95 AAAA ATOM 2929 C LYS A 3665 9.071 26.421 70.818 1.00 31.95 AAAA ATOM 2931 CA ASP A 366 7.919 27.136 69.012 1.00 32.75 AAAA ATOM 2931 CA ASP A 366 7.919 27.136 69.012 1.00 32.75 AAAA ATOM 2931 CA ASP A 366 7.919 27.136 69.012 1.00 32.94 AAAA ATOM 2931 CA ASP A 366 7.919 27.136 69.012 1.00 32.94 AAAA ATOM 2931 CA ASP A 366 7.919 27.136 69.012 1.00 32.94 AAAA ATOM 2931 CA ASP A 366 9.130 25.767 69.01 1.00 32.95 AAAA ATOM 2931 CA ASP A 366 9.130 25.767 69.01 1.00 32.95 AAAA ATOM 2931 CA ASP A 366 9.100 25.767 69.01 1.00 32.77 AAAA ATOM 2935 CD ASP A 366 9.130 25.767 69.01 1.00 32.95 AAAA ATOM 2935 CD ASP A 366 9.130 25.767 69.01 1.00 32.95 AAAA ATOM 2935 CD ASP A 366 9.130 25.767 69.01 1.00 32.95 AAAA ATOM 2935 CD ASP A 366 9.130 25.767 69.01 1.00 32.95 AAAA ATOM 2935 CD ASP A 366 9.100 25.767 69.90 1.00 32.77 AAAA ATOM 2935 CD ASP A 366 9.100 25.767 69.90 1.00 32.77 AAAA ATOM 2935 CD ASP A 366 9.100 25.767 69.90 1.00 32.77 AAAA ATOM 2935 CD ASP A 366 9.100 25.767 69.90 1.00 | MOTA | | | | | | | | | |
| ATOM 2918 CG2 VAL A 364 11.739 31.722 68 162 - 1.00 34.13 AAAA ATOM 2919 C VAL A 364 9.908 29.499 68.370 1.00 31.44 AAAA ATOM 2919 C VAL A 364 9.908 29.499 68.370 1.00 34.44 AAAA ATOM 2920 O VAL A 365 8.980 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.980 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CG LYS A 365 8.970 28.790 70.476 1.00 34.28 AAAA ATOM 2924 CG LYS A 365 8.307 30.705 72.033 1.00 34.65 AAAA ATOM 2925 CD LYS A 365 7.868 29.319 71.508 1.00 34.28 AAAA ATOM 2926 CE LYS A 365 7.282 31.881 73.039 1.00 34.85 AAAA ATOM 2927 NZ LYS A 365 7.282 31.881 73.039 1.00 34.85 AAAA ATOM 2928 C LYS A 365 7.282 31.881 73.039 1.00 34.85 AAAA ATOM 2928 C LYS A 365 8.504 7.282 31.881 70.00 37.91 AAAA ATOM 2928 C LYS A 365 8.544 77.342 70.109 1.00 37.91 AAAA ATOM 2928 C LYS A 3665 8.544 27.342 70.109 1.00 32.75 AAAA ATOM 2928 C LYS A 3665 8.544 27.342 70.109 1.00 32.75 AAAA ATOM 2928 C LYS A 3665 8.544 27.342 70.109 1.00 32.75 AAAA ATOM 2930 N ASP A 3666 7.600 25.777 68.581 1.00 31.95 AAAA ATOM 2931 CA ASP A 3666 7.600 25.777 68.581 1.00 31.95 AAAA ATOM 2932 CB ASP A 3666 6.459 25.726 67.557 1.00 33.98 AAAA ATOM 2933 CG ASP A 366 6.459 25.766 68.307 1.00 33.98 AAAA ATOM 2935 ODZ ASP A 366 6.459 25.766 68.307 1.00 33.98 AAAA ATOM 2936 C ASP A 366 4.870 25.776 68.307 1.00 33.98 AAAA ATOM 2937 O ASP A 366 4.870 25.776 68.307 1.00 33.98 AAAA ATOM 2938 N THR 367 9.473 25.959 67.012 1.00 33.05 AAAA ATOM 2938 O TAR ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2939 O LY ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2931 O ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2932 CB ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2934 ODI ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2935 O C ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2936 C ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2937 O ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2936 C ASP A 366 8.820 25.757 69.307 1.00 33.29 AAAA ATOM 2936 C ASP A 366 8.820 25.800 69.950 1.00 32.77 AAAA ATOM 2940 CB THR A 367 12.711 26.377 65.16 | MOTA | | | | | | | | | |
| ATOM 2918 CC2 VAL A 364 19.98 29.499 68.370 1.00 31.83 AAAA ATOM 2919 C VAL A 364 9.996 29.499 68.370 1.00 34.44 AAAA ATOM 2920 C VAL A 364 10.789 28.640 68.430 1.00 36.01 -AAAA ATOM 2921 N LYS A 365 8.980 29.649 69.305 1.00 33.20 AAAAA ATOM 2922 CA LYS A 365 8.980 29.649 69.305 1.00 33.20 AAAAA ATOM 2923 CB LYS A 365 8.980 70.28.790 70.476 1.00 34.28 AAAA ATOM 2924 CG LYS A 365 7.968 29.319 71.508 1.00 33.20 AAAAA ATOM 2925 CD LYS A 365 7.968 29.319 71.508 1.00 33.20 AAAAA ATOM 2925 CD LYS A 365 7.968 32.534 73.638 1.00 34.28 AAAA ATOM 2926 CE LYS A 365 7.628 31.181 73.039 1.00 33.67 AAAA ATOM 2927 NZ LYS A 365 7.628 32.534 73.638 1.00 36.47 AAAA ATOM 2928 C LYS A 365 8.854 27.342 70.109 1.00 32.75 AAAAA ATOM 2929 O LYS A 365 8.854 27.342 70.109 1.00 32.75 AAAAA ATOM 2929 O LYS A 365 8.854 27.342 70.109 1.00 32.75 AAAAA ATOM 2929 O LYS A 366 7.919 27.136 69.012 1.00 32.81 AAAA ATOM 2931 CA ASP A 366 7.919 27.136 69.012 1.00 33.81 AAAA ATOM 2931 CA ASP A 366 7.919 27.136 69.012 1.00 33.98 AAAA ATOM 2932 CB ASP A 366 6.459 25.777 68.581 1.00 33.98 AAAA ATOM 2933 CG ASP A 366 6.459 25.777 68.581 1.00 33.98 AAAA ATOM 2933 CG ASP A 366 6.459 25.776 69.307 1.00 33.98 AAAA ATOM 2934 ODI ASP A 366 6.459 25.776 69.307 1.00 33.98 AAAA ATOM 2935 OD2 ASP A 366 6.430 25.777 69.307 1.00 33.99 AAAAA ATOM 2935 CG ASP A 366 8.820 25.167 69.307 1.00 33.99 AAAAA ATOM 2936 C ASP A 366 8.820 25.167 69.907 1.00 33.99 AAAAA ATOM 2937 O ASP A 366 8.820 25.167 69.907 1.00 33.99 AAAAA ATOM 2937 O ASP A 366 8.820 25.167 69.907 1.00 33.99 AAAAA ATOM 2937 C ASP A 366 8.820 25.167 69.907 1.00 33.99 AAAAA ATOM 2937 C ASP A 366 8.820 25.167 69.907 1.00 33.99 AAAAA ATOM 2937 C ASP A 366 8.820 25.167 69.907 1.00 33.99 AAAAA ATOM 2939 C C THR A 367 11.309 25.500 66.412 1.00 32.27 AAAA ATOM 2940 CB THR A 367 11.309 25.500 66.412 1.00 32.27 AAAA ATOM 2940 CB THR A 367 11.309 25.500 66.412 1.00 32.27 AAAA ATOM 2950 CC CUT HR A 367 11.309 25.500 66.412 1.00 32.27 AAAA ATOM 2954 CC LEU A 368 11.309 69.900 69.900 1.00 32.71 AAAA ATOM 2955 CG CLU A 36 | ATOM | 2916 | _ | | | | | | | |
| ATOM 2919 C VAL A 364 9.908 29.499 68.370 1.00 34.44 AAAA ATOM 2921 N LYS A 365 8.980 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.980 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CCA LYS A 365 8.970 28.790 70.476 1.00 33.27 AAAA ATOM 2923 CB LYS A 365 7.968 29.319 71.508 1.00 34.28 AAAA ATOM 2924 CC LYS A 365 7.968 29.319 71.508 1.00 34.28 AAAA ATOM 2925 CD LYS A 365 7.282 31.181 73.039 1.00 34.85 AAAA ATOM 2926 CE LYS A 365 7.282 31.181 73.039 1.00 34.85 AAAA ATOM 2926 CE LYS A 365 7.658 32.534 73.638 1.00 36.47 AAAA ATOM 2926 CE LYS A 365 6.698 32.990 74.710 1.00 37.91 AAAA ATOM 2928 C LYS A 365 9.071 26.421 70.818 1.00 31.75 AAAA ATOM 2929 O LYS A 365 9.071 26.421 70.818 1.00 31.75 AAAA ATOM 2930 N ASP A 366 7.500 25.777 68.581 1.00 33.87 AAAA ATOM 2931 CA ASP A 366 7.500 25.777 68.581 1.00 33.98 AAAA ATOM 2932 CB ASP A 366 6.459 25.726 67.557 1.00 33.98 AAAA ATOM 2933 CC BASP A 366 5.439 25.726 67.557 1.00 33.98 AAAA ATOM 2934 OD1 ASP A 366 7.500 25.777 68.581 1.00 33.98 AAAA ATOM 2934 OD1 ASP A 366 4.332 26.722 67.412 1.00 33.98 AAAA ATOM 2935 CD ASP A 366 4.332 26.722 67.412 1.00 33.98 AAAA ATOM 2935 C ASP A 366 8.820 25.767 69.307 1.00 33.98 AAAA ATOM 2935 C ASP A 366 4.332 26.722 67.412 1.00 33.05 AAAA ATOM 2935 C ASP A 366 8.820 25.767 69.307 1.00 33.05 AAAA ATOM 2937 C ASP A 366 8.820 25.767 69.307 1.00 33.05 AAAA ATOM 2937 C ASP A 366 8.820 25.767 69.307 1.00 33.05 AAAA ATOM 2937 C ASP A 366 8.820 25.767 69.307 1.00 33.05 AAAA ATOM 2937 C ASP A 366 8.820 25.767 69.900 1.00 32.27 AAAA ATOM 2937 C ASP A 366 8.820 25.767 69.900 1.00 32.27 AAAA ATOM 2937 C ASP A 366 8.820 25.767 69.900 1.00 32.27 AAAA ATOM 2934 C C LYR A 367 11.304 26.719 65.641 1.00 33.22 AAAA ATOM 2930 C ASP A 366 8.820 25.767 69.900 1.00 32.27 AAAA ATOM 2930 C ASP A 366 8.820 25.767 69.900 1.00 32.27 AAAA ATOM 2930 C ASP A 366 8.820 25.767 69.900 1.00 32.27 AAAA ATOM 2930 C ASP A 366 8.820 25.767 69.900 1.00 32.27 AAAA ATOM 2930 C ASP A 366 8.820 25.767 69.900 1.00 32.27 AAAA ATOM 2930 C ASP A 366 8.820 25.800 69.900 1.00 32.27 | ATOM · | 2917 | | | | | | | • | , |
| ATOM 2921 N LYS A 365 | MOTA | 2918 | CG2 | | | | | | | |
| ATOM 2921 N LYS A 365 8.980 29.649 69.305 1.00 33.27 AAAA ATOM 2922 CA LYS A 365 8.970 28.790 70.476 1.00 33.20 AAAA ATOM 2923 CB LYS A 365 7.968 29.319 71.508 1.00 34.28 AAAA ATOM 2924 CG LYS A 365 7.282 31.181 73.039 1.00 34.28 AAAA ATOM 2926 CE LYS A 365 7.282 31.181 73.039 1.00 34.85 AAAA ATOM 2926 CE LYS A 365 7.282 31.181 73.039 1.00 34.85 AAAA ATOM 2926 CE LYS A 365 7.588 32.990 74.710 1.00 37.91 AAAA ATOM 2928 C LYS A 365 6.698 32.990 74.710 1.00 37.91 AAAA ATOM 2928 C LYS A 365 9.071 26.421 70.818 1.00 31.95 AAAA ATOM 2929 0 LYS A 365 9.071 26.421 70.818 1.00 31.95 AAAA ATOM 2930 N ASP A 366 7.600 25.777 68.581 1.00 33.65 AAAA ATOM 2931 CA ASP A 366 7.600 25.777 68.581 1.00 33.65 AAAA ATOM 2931 CA ASP A 366 7.600 25.777 68.581 1.00 33.98 AAAA ATOM 2933 CG ASP A 366 5.131 26.107 68.140 1.00 33.98 AAAA ATOM 2933 CG ASP A 366 5.131 26.107 68.140 1.00 33.98 AAAA ATOM 2934 0D1 ASP A 366 4.870 25.766 69.307 1.00 33.89 AAAA ATOM 2935 C ASP A 366 5.131 26.107 68.140 1.00 33.98 AAAA ATOM 2935 C ASP A 366 8.820 25.767 69.307 1.00 33.89 AAAA ATOM 2935 C ASP A 366 8.820 25.767 69.307 1.00 33.89 AAAA ATOM 2935 C ASP A 366 8.820 25.767 69.307 1.00 33.89 AAAA ATOM 2935 C ASP A 366 8.820 25.767 69.307 1.00 33.05 AAAA ATOM 2937 C ASP A 366 8.820 25.167 67.940 1.00 33.98 AAAA ATOM 2937 C ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2937 C ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2937 C ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2937 C ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2939 CA THR A 367 10.0684 25.740 66.412 1.00 32.27 AAAA ATOM 2939 CA THR A 367 10.0684 25.740 66.412 1.00 32.28 AAAA ATOM 2940 CB THR A 367 10.473 27.703 64.520 1.00 33.07 AAAA ATOM 2940 CB THR A 367 10.473 27.703 64.920 1.00 33.07 AAAA ATOM 2943 CC THR A 367 10.473 27.703 69.900 1.00 32.27 AAAA ATOM 2940 CB THR A 367 10.473 27.703 69.900 1.00 32.27 AAAA ATOM 2940 CB THR A 367 10.473 27.703 69.900 1.00 32.27 AAAA ATOM 2940 CB LEU A 368 12.886 25.560 69.482 1.00 32.27 AAAA ATOM 2950 CC LEU A 368 12.886 25.560 69.900 | ATOM | 2919 | С | VAL A | 364 | | | | | |
| ATOM 2923 CB LYS A 365 | MOTA | 2920 | 0 | VAL A | 364 | | | | | |
| ATOM 2923 CB LYS A 365 | ATOM | 2921 | N | | | | | | | |
| ATOM 2925 CG LYS A 365 7.282 31.181 73.03 1.00 33.67 AAAA ATOM 2926 CE LYS A 365 7.282 31.181 73.03 1.00 34.85 AAAA ATOM 2927 NZ LYS A 365 7.658 32.534 73.638 1.00 36.47 AAAA ATOM 2928 C LYS A 365 7.658 32.534 73.638 1.00 36.47 AAAA ATOM 2928 C LYS A 365 8.659 32.990 74.710 1.00 37.75 AAAA ATOM 2928 C LYS A 365 8.658 27.342 70.100 1.00 32.75 AAAA ATOM 2929 O LYS A 365 8.654 27.342 70.100 1.00 32.75 AAAA ATOM 2929 O LYS A 366 7.900 25.777 68.581 1.00 31.95 AAAA ATOM 2931 CA ASP A 366 7.900 25.777 68.581 1.00 33.65 AAAA ATOM 2931 CA ASP A 366 6.659 25.726 67.557 1.00 33.98 AAAA ATOM 2931 CA ASP A 366 6.559 25.726 67.557 1.00 33.98 AAAA ATOM 2933 CG ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2933 CG ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2935 CD ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2935 CD ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2935 CD ASP A 366 4.870 25.767 69.307 1.00 33.08 AAAA ATOM 2935 CD ASP A 366 4.322 26.722 67.412 1.00 35.08 AAAA ATOM 2935 CD ASP A 366 9.140 24.006 68.172 1.00 33.05 AAAA ATOM 2937 O ASP A 366 9.140 24.006 68.172 1.00 33.05 AAAA ATOM 2938 N THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2939 CA THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2939 CA THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2940 CB THR A 367 11.304 26.719 65.641 1.00 32.28 AAAA ATOM 2940 CT THR A 367 12.711 26.377 65.166 1.00 33.29 AAAA ATOM 2940 CB THR A 367 12.712 26.377 69.4520 1.00 30.64 AAAA ATOM 2947 CB LEU A 368 11.555 25.806 69.482 1.00 32.27 AAAA ATOM 2940 CB THR A 367 12.712 23.918 67.352 1.00 30.64 AAAA ATOM 2947 CB LEU A 368 12.888 25.560 69.482 1.00 32.27 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG CEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG CEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD LEU A 368 13.086 33.099 27.309 64.520 1.00 30.64 AAAA ATOM 2950 CD LEU A 368 13.089 20.25 5.00 69.482 1.00 33.89 AAAA ATOM 2955 CB GU A 369 69.91 20.589 39 39 68.597 1.00 31.86 AAAA ATOM 2950 CC GU A | ATOM | 2922 | CA | LYS A | 365 | | | | | |
| ATOM 2925 CD LYS A 365 7.282 31.181 73.033 1.00 33.67 AAAA ATOM 2926 CE LYS A 365 7.658 32.534 73.638 1.00 36.47 AAAA ATOM 2927 NZ LYS A 365 6.688 32.990 74.710 1.00 37.91 AAAA ATOM 2928 C LYS A 365 6.688 32.990 74.710 1.00 37.91 AAAA ATOM 2928 C LYS A 365 6.688 32.990 74.710 1.00 37.91 AAAA ATOM 2929 O LYS A 365 9.071 26.421 70.818 1.00 31.95 AAAA ATOM 2929 O LYS A 365 9.071 26.421 70.818 1.00 31.95 AAAA ATOM 2921 CA ASP A 366 7.500 25.777 68.581 1.00 32.81 AAAA ATOM 2931 CA ASP A 366 7.500 25.777 68.581 1.00 33.65 AAAA ATOM 2931 CA ASP A 366 6.459 25.767 69.307 1.00 33.98 AAAA ATOM 2933 CG ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2934 ODI ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2935 ODZ ASP A 366 4.332 26.722 67.412 1.00 35.08 AAAA ATOM 2935 ODZ ASP A 366 8.20 25.167 67.940 1.00 33.05 AAAA ATOM 2937 O ASP A 366 8.20 25.167 67.940 1.00 33.05 AAAA ATOM 2937 O ASP A 366 8.20 25.167 67.940 1.00 33.05 AAAA ATOM 2937 O ASP A 366 8.20 25.167 67.940 1.00 33.05 AAAA ATOM 2937 O ASP A 366 8.20 25.167 67.940 1.00 33.05 AAAA ATOM 2937 O THR A 367 9.473 25.959 67.102 1.00 33.07 AAAA ATOM 2939 CA THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2930 CT THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2940 CE THR A 367 10.473 27.039 64.520 1.00 30.64 AAAA ATOM 2940 CE THR A 367 11.304 26.719 65.641 1.00 32.27 AAAA ATOM 2942 CG2 THR A 367 11.680 25.044 67.442 1.00 31.71 AAAA ATOM 2943 C CG THR A 367 12.711 26.377 65.166 1.00 32.27 AAAA ATOM 2943 C CG THR A 367 12.712 26.377 69.969 1.00 30.45 AAAA ATOM 2945 C CG THR A 367 12.712 23.918 67.352 1.00 30.45 AAAA ATOM 2945 C CG C THR A 367 12.712 23.918 67.352 1.00 30.45 AAAA ATOM 2945 C CG C THR A 367 12.712 23.918 67.352 1.00 30.45 AAAA ATOM 2945 C CG C THR A 367 12.712 23.918 67.352 1.00 30.45 AAAA ATOM 2945 C CG C THR A 367 12.712 23.918 67.352 1.00 30.45 AAAA ATOM 2945 C CG C C C C C C C C C C C C C C C C C | ATOM | 2923 | CB | LYS A | 365 | | 29.319 | | | |
| ATOM 2926 CE LYS A 365 | | 2924 | CG | LYS A | 365 | 8.307 | 30.705 | 72.033 | 1.00 33.67 | |
| ATOM 2926 CE LYS A 365 | | 2925 | CD | LYS A | 365 | 7.282 | 31.181 | 73.039 | 1.00 34.85 | |
| ATOM 2928 C LYS A 365 6.698 32.990 74.710 1.00 37.91 AAAA ATOM 2929 C LYS A 365 8.654 27.342 70.109 1.00 32.75 AAAA ATOM 2929 N ASP A 366 7.919 27.136 69.012 1.00 31.95 AAAA ATOM 2931 CA ASP A 366 7.919 27.136 69.012 1.00 33.65 AAAA ATOM 2932 CB ASP A 366 7.919 27.136 69.012 1.00 33.65 AAAA ATOM 2933 CG ASP A 366 5.131 26.107 68.581 1.00 33.94 AAAA ATOM 2933 CG ASP A 366 5.131 26.107 68.140 1.00 33.94 AAAA ATOM 2933 CD ASP A 366 4.870 25.767 69.307 1.00 33.99 AAAA ATOM 2935 OD2 ASP A 366 4.870 25.767 69.307 1.00 33.99 AAAA ATOM 2935 OD2 ASP A 366 8.820 25.167 69.307 1.00 33.05 AAAA ATOM 2936 C ASP A 366 8.820 25.167 69.307 1.00 33.05 AAAA ATOM 2937 O ASP A 366 8.820 25.167 69.307 1.00 33.05 AAAA ATOM 2937 O ASP A 366 9.140 24.006 68.172 1.00 33.05 AAAA ATOM 2938 N THR A 367 9.473 25.959 67.102 1.00 33.05 AAAA ATOM 2939 CA THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2940 CB THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2941 OG1 THR A 367 10.473 27.039 64.520 1.00 30.64 AAAA ATOM 2941 OG1 THR A 367 12.711 26.377 65.166 1.00 32.28 AAAA ATOM 2944 C THR A 367 12.711 26.377 65.166 1.00 32.27 AAAA ATOM 2944 C THR A 368 11.955 25.896 68.422 1.00 30.64 AAAA ATOM 2945 C THR A 368 13.005 26.749 70.421 1.00 32.27 AAAA ATOM 2946 C A LEU A 368 12.178 23.918 67.352 1.00 30.54 AAAA ATOM 2946 C A LEU A 368 12.188 25.560 69.482 1.00 32.07 AAAA ATOM 2947 CB LEU A 368 12.188 27.170 69.899 1.00 32.07 AAAA ATOM 2947 CB LEU A 368 13.005 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.005 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.005 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.205 26.749 70.421 1.00 32.05 AAAA ATOM 2950 CD2 LEU A 368 13.005 26.749 70.421 1.00 32.05 AAAA ATOM 2950 CD2 LEU A 368 13.206 23.133 70.049 1.00 31.86 AAAA ATOM 2950 CD2 LEU A 368 13.206 23.133 70.049 1.00 31.86 AAAA ATOM 2950 CD2 LEU A 368 13.206 23.133 70.375 1.00 31.86 AAAA ATOM 2950 CD2 LEU A 369 9.211 23.319 71.748 1.00 31.30 AAAA ATOM 2950 CD LEU A 369 9.211 23.319 71.748 1.00 31.30 AAAA ATOM 2950 CD2 LEU | | | CE | LYS A | 365 | 7.658 | 32.534 | 73.638 | | |
| ATOM 2928 C LYS A 365 8.654 27.342 70.109 1.00 32.75 AAAA ATOM 2930 N ASP A 366 7.919 27.136 69.012 1.00 31.95 AATOM 2931 CA ASP A 366 7.600 25.777 68.581 1.00 33.98 ATOM 2932 CB ASP A 366 6.459 25.726 67.557 1.00 33.98 ATOM 2933 CG ASP A 366 6.459 25.726 67.557 1.00 33.98 ATOM 2934 ODI ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2935 CD ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2936 CD ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2937 CD ASP A 366 8.820 25.167 67.940 1.00 33.98 AAAA ATOM 2938 N THR A 367 9.473 25.959 67.102 1.00 33.05 AAAA ATOM 2938 N THR A 367 10.684 25.540 66.412 1.00 33.07 AAAA ATOM 2939 CA THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2940 CB THR A 367 11.304 26.719 65.641 1.00 32.27 AAAA ATOM 2941 OGI THR A 367 12.711 26.377 65.166 1.00 30.64 AAAA ATOM 2942 CG2 THR A 367 12.711 26.377 65.166 1.00 30.64 AAAA ATOM 2944 C THR A 367 12.712 26.377 65.166 1.00 30.45 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 31.71 AAAA ATOM 2946 CA LEU A 368 11.955 25.896 68.426 1.00 32.27 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 C CLEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2946 CA LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 C CLEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.266 23.133 70.489 1.00 32.49 ATOM 2951 C LEU A 368 13.266 23.133 70.489 1.00 32.27 AAAA ATOM 2952 C CD2 LEU A 368 13.266 23.133 70.489 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 369 13.266 23.133 70.489 1.00 32.71 AAAA ATOM 2950 CD2 LEU A 368 13.266 23.133 70.489 1.00 32.71 AAAA ATOM 2950 CD2 LEU A 368 13.266 23.133 70.489 1.00 33.82 ATOM 2950 CD2 LEU A 369 9.211 23.319 71.748 1.00 32.77 AAAA ATOM 2950 CD GUU A 369 9.211 23.319 71.748 1.00 37.00 41.56 ATOM 2950 CD GUU A 369 9.211 23.319 71.748 1.00 37.00 41.56 ATOM 2950 CD GUU A 369 10.687 23.135 71.375 1.00 34.56 AAAA ATOM 2950 CD GUU A 369 10.056 20.050 65.775 1.00 41.56 AAAA ATOM 2960 C LYS A 370 10.566 20.000 65.775 | | | NZ | LYS A | 365 | 6.698 | 32.990 | 74.710 | 1.00 37.91 | |
| ATOM 2930 O LYS A 365 9.071 26.421 70.818 1.00 31.95 AAAA ATOM 2931 CA ASP A 366 7.919 27.136 69.012 1.00 32.81 AAAA ATOM 2931 CA ASP A 366 7.600 25.777 68.581 1.00 33.65 AAAA ATOM 2932 CB ASP A 366 6.459 25.726 67.557 1.00 33.98 AAAA ATOM 2933 CG ASP A 366 6.459 25.726 67.557 1.00 33.98 AAAA ATOM 2934 ODI ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2935 ODZ ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2936 C ASP A 366 4.870 25.767 69.307 1.00 33.99 AAAA ATOM 2936 C ASP A 366 9.140 24.006 68.140 1.00 33.05 AAAA ATOM 2937 O ASP A 366 9.140 24.006 68.172 1.00 33.05 AAAA ATOM 2937 O ASP A 366 9.140 24.006 68.172 1.00 33.07 AAAA ATOM 2938 N THR A 367 9.473 25.959 67.102 1.00 33.07 AAAA ATOM 2939 CA THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2940 CB THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2940 CB THR A 367 10.473 27.039 64.520 1.00 30.64 AAAA ATOM 2941 OGI THR A 367 12.711 26.377 65.166 1.00 32.28 AAAA ATOM 2942 CGZ THR A 367 12.711 26.377 65.166 1.00 33.29 AAAA ATOM 2943 C THR A 367 12.178 23.918 67.352 1.00 30.45 AAAA ATOM 2944 C THR A 368 11.955 25.896 68.426 1.00 32.28 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.27 AAAA ATOM 2945 C LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG LEU A 368 13.085 26.749 70.421 1.00 32.271 AAAA ATOM 2950 CDZ LEU A 368 13.085 26.749 70.421 1.00 32.271 AAAA ATOM 2950 CDZ LEU A 368 13.085 26.749 70.421 1.00 32.271 AAAA ATOM 2950 CDZ LEU A 368 13.085 26.749 70.421 1.00 32.271 AAAA ATOM 2950 CDZ LEU A 368 13.085 26.749 70.421 1.00 32.271 AAAA ATOM 2950 CDZ LEU A 368 13.085 26.749 70.421 1.00 32.271 AAAA ATOM 2950 CDZ LEU A 368 13.085 26.749 70.421 1.00 32.271 AAAA ATOM 2950 CDZ LEU A 368 13.085 26.749 70.421 1.00 33.82 AAAA ATOM 2950 CDZ LEU A 368 13.266 23.133 70.08 A68 6.597 1.00 31.86 AAAA ATOM 2950 CDZ LEU A 368 13.266 23.133 70.489 1.00 31.00 AAAA ATOM 2950 CDZ LEU A 368 13.266 23.133 70.489 1.00 31.86 AAA | | | С | LYS ? | 365 | 8.654 | 27.342 | 70.109 | 1.00 32.75 | AAAA |
| ATOM 2931 CA ASP A 366 7.919 27.136 69.012 1.00 32.81 AAAA ATOM 2932 CB ASP A 366 6.459 25.727 68.581 1.00 33.65 AAAA ATOM 2933 CG ASP A 366 5.131 26.107 68.140 1.00 33.98 AAAA ATOM 2933 CG ASP A 366 5.131 26.107 68.140 1.00 33.94 AAAA ATOM 2935 OD2 ASP A 366 4.870 25.767 69.307 1.00 33.89 AAAA ATOM 2935 OD2 ASP A 366 4.332 26.722 67.412 1.00 35.08 AAAA ATOM 2936 C ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2937 O ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2937 O ASP A 366 9.140 24.006 68.172 1.00 33.66 AAAA ATOM 2938 N THR A 367 9.473 25.959 67.102 1.00 33.07 AAAA ATOM 2939 CA THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2939 CA THR A 367 11.304 26.719 65.641 1.00 32.28 AAAA ATOM 2941 OG1 THR A 367 10.473 27.039 64.520 1.00 33.07 AAAA ATOM 2941 OG1 THR A 367 11.304 26.719 65.641 1.00 32.28 AAAA ATOM 2942 CG2 THR A 367 11.680 25.044 67.442 1.00 31.71 AAAA ATOM 2943 C THR A 367 11.680 25.044 67.442 1.00 31.71 AAAA ATOM 2944 O THR A 367 11.680 25.044 67.442 1.00 31.71 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.49 AAAA ATOM 2946 CA LEU A 368 11.955 25.896 68.426 1.00 32.49 AAAA ATOM 2946 CA LEU A 368 12.888 25.560 69.482 1.00 32.47 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2949 CD1 LEU A 368 13.095 26.749 70.421 1.00 32.27 AAAA ATOM 2949 CD1 LEU A 368 13.095 26.749 70.421 1.00 32.27 AAAA ATOM 2949 CD1 LEU A 368 13.095 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.095 26.749 70.421 1.00 32.27 AAAA ATOM 2955 C G GLU A 369 10.687 23.135 71.00 30.30 AAAA ATOM 2955 C CD2 LEU A 368 12.455 24.334 70.256 1.00 33.00 AAAA ATOM 2955 C CD2 LEU A 368 12.455 24.334 70.256 1.00 33.00 AAAA ATOM 2955 C G GLU A 369 10.687 23.135 71.375 1.00 36.07 AAAA ATOM 2955 C G GLU A 369 10.687 23.135 71.375 1.00 36.07 AAAA ATOM 2955 C G GLU A 369 10.687 23.135 71.00 31.86 AAAA ATOM 2956 C G GLU A 369 10.687 23.135 71.00 31.86 AAAA ATOM 2957 C C GLU A 369 6.957 25.489 73.341 1.00 41.56 AAAA ATOM 2957 C C GLU A 369 10.689 21.282 70.661 1.00 37.16 AAAA ATOM 2960 C GLU A 36 | | | | LYS A | 365 | 9.071 | 26.421 | 70.818 | 1.00 31.95 | AAAA |
| ATOM 2931 CA ASP A 366 7.600 25.777 68.581 1.00 33.65 AAAA ATOM 2932 CB ASP A 366 5.131 26.107 68.140 1.00 33.94 AAAA ATOM 2934 ODI ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2935 ODZ ASP A 366 4.870 25.767 69.307 1.00 33.98 AAAA ATOM 2936 C ASP A 366 8.820 25.167 67.940 1.00 35.08 AAAA ATOM 2937 O ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2938 N THR A 367 9.140 24.006 68.172 1.00 33.05 AAAA ATOM 2938 N THR A 367 9.140 25.959 67.102 1.00 33.07 AAAA ATOM 2939 CA THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2930 CB THR A 367 10.684 25.540 66.412 1.00 32.28 AAAA ATOM 2940 CB THR A 367 10.473 27.039 64.520 1.00 33.64 AAAA ATOM 2941 CG THR A 367 10.473 27.039 64.520 1.00 33.64 AAAA ATOM 2942 CG THR A 367 11.680 25.044 67.442 1.00 31.29 AAAA ATOM 2944 C THR A 367 12.178 23.918 67.352 1.00 30.64 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.27 AAAA ATOM 2946 C LEU A 368 11.955 25.896 68.426 1.00 32.20 AAAA ATOM 2947 CB LEU A 368 11.955 25.896 68.426 1.00 32.27 AAAA ATOM 2948 CG LEU A 368 12.888 25.560 69.482 1.00 32.27 AAAA ATOM 2949 CD LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.085 26.749 70.421 1.00 32.71 AAAA ATOM 2950 CD2 LEU A 368 13.085 26.749 70.421 1.00 32.71 AAAA ATOM 2950 CD2 LEU A 368 13.085 26.749 70.421 1.00 32.71 AAAA ATOM 2950 CD2 LEU A 368 13.085 26.749 70.421 1.00 32.71 AAAA ATOM 2950 CD2 LEU A 368 13.085 26.749 70.421 1.00 32.71 AAAA ATOM 2950 CD2 LEU A 368 13.709 28 393 68.597 1.00 31.86 AAAA ATOM 2950 CD2 LEU A 368 13.709 28 393 68.597 1.00 31.86 AAAA ATOM 2950 CD2 LEU A 368 15.488 27.170 69.899 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 369 10.697 27.809 69.960 1.00 37.00 AAAA ATOM | | | | ASP A | 366 | 7.919 | 27.136 | 69.012 | 1.00 32.81 | AAAA |
| ATOM 2932 CB ASP A 366 | | | | ASP A | 366 | 7.600 | 25.777 | 68.581 | 1.00 33.65 | AAAA |
| ATOM 2933 CG ASP A 366 5.131 26.107 68.140 1.00 33.94 AAAA ATOM 2934 OD1 ASP A 366 4.870 25.767 69.307 1.00 33.89 AAAA ATOM 2935 OD2 ASP A 366 4.870 25.767 69.307 1.00 33.05 AAAA ATOM 2936 C ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2937 O ASP A 366 9.140 24.006 68.172 1.00 33.06 AAAA ATOM 2938 N THR A 367 9.473 25.959 67.102 1.00 33.07 AAAA ATOM 2939 CA THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2940 CB THR A 367 10.473 27.039 64.520 1.00 32.27 AAAA ATOM 2940 CB THR A 367 10.473 27.039 64.520 1.00 30.64 AAAA ATOM 2942 CG2 THR A 367 12.711 26.377 65.166 1.00 32.28 AAAA ATOM 2942 CG2 THR A 367 11.680 25.044 67.492 1.00 31.71 AAAA ATOM 2943 C THR A 367 12.178 23.918 67.352 1.00 30.45 AAAA ATOM 2943 C THR A 367 12.178 23.918 67.352 1.00 30.45 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.49 AAAA ATOM 2946 CA LEU A 368 11.955 25.896 68.426 1.00 32.27 AAAA ATOM 2947 CB LEU A 368 12.888 25.560 69.482 1.00 32.49 AAAA ATOM 2949 CD1 LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2949 CD1 LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2949 CD1 LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.266 23.133 70.489 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 12.455 24.334 70.256 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 12.455 24.334 70.256 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2950 CD2 LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2950 CD2 LEU A 368 13.266 23.133 70.489 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.266 23.133 70.489 1.00 31.82 AAAA ATOM 2950 CD2 LEU A 368 12.455 24.334 70.256 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 12.455 24.334 70.256 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 12.455 24.334 70.256 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 12.455 24.334 70.256 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 12.455 24.334 70.256 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 369 6.917 23.256 CD2 AAAA ATOM 2950 CD2 LEU A 369 6.917 23.256 CD2 AAAA ATOM 2950 CD2 LEU A 369 6. | | _ | | | | 6.459 | 25.726 | 67.557 | 1.00 33.98 | AAAA |
| ATOM 2934 OD1 ASP A 366 | | _ | | | | 5.131 | 26,107 | 68.140 | 1.00 33.94 | AAAA |
| ATOM 2935 OD2 ASP A 366 | | | | ASP A | 366 | 4.870 | 25.767 | 69.307 | 1.00 33.89 | AAAA |
| ATOM 2936 C ASP A 366 8.820 25.167 67.940 1.00 33.05 AAAA ATOM 2938 N THR A 367 9.473 25.959 67.102 1.00 33.07 AAAA ATOM 2938 N THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2940 CB THR A 367 11.304 26.719 65.641 1.00 32.27 AAAA ATOM 2941 CG1 THR A 367 10.473 27.039 64.520 1.00 30.64 AAAA ATOM 2942 CG2 THR A 367 12.711 26.377 65.166 1.00 33.29 AAAA ATOM 2942 CG2 THR A 367 12.711 26.377 65.166 1.00 33.29 AAAA ATOM 2944 C THR A 367 12.712 26.377 65.166 1.00 33.29 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 31.71 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.05 AAAA ATOM 2945 C LEU A 368 11.955 25.896 69.482 1.00 32.04 AAAA ATOM 2946 CG LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG LEU A 368 14.097 27.889 69.960 1.00 32.71 AAAA ATOM 2949 CD1 LEU A 368 14.097 27.889 69.960 1.00 32.71 AAAA ATOM 2949 CD1 LEU A 368 15.488 27.170 69.899 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.709 28.393 68.597 1.00 31.86 AAAA ATOM 2950 CD2 LEU A 368 13.709 28.393 68.597 1.00 31.86 AAAA ATOM 2950 CD2 LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2950 CD2 LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2955 CB GIU A 369 11.183 24.285 70.645 1.00 34.30 AAAA ATOM 2955 CB GIU A 369 10.687 23.315 71.375 1.00 36.07 AAAA ATOM 2955 CB GIU A 369 10.687 23.315 71.375 1.00 34.29 AAAA ATOM 2955 CB GIU A 369 10.687 23.315 71.375 1.00 34.29 AAAA ATOM 2955 CB GIU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2955 CB GIU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2955 CB GIU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2955 CB GIU A 369 10.687 23.315 71.375 1.00 37.71 AAAA ATOM 2955 CB GIU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2955 CB GIU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2956 CG GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2956 CG GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2956 CG GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2966 CB LYS A 370 6.000 10.797 20.547 68.557 1.00 37.71 AAAA ATOM 2966 CD LYS A 370 6.000 10.797 20.547 68.557 1.00 41.54 AAAA AT | | | | | | 4.332 | 26.722 | 67.412 | 1.00 35.08 | AAAA |
| ATOM 2937 O ASP A 366 9.140 24.006 68.172 1.00 33.66 AAAA ATOM 2938 N THR A 367 10.684 25.550 67.102 1.00 33.07 AAAA ATOM 2940 CB THR A 367 11.304 26.719 65.641 1.00 32.28 AAAA ATOM 2941 OGI THR A 367 11.304 26.719 65.641 1.00 32.28 AAAA ATOM 2941 CGZ THR A 367 12.711 26.377 65.166 1.00 33.29 AAAA ATOM 2942 CGZ THR A 367 12.711 26.377 65.166 1.00 33.29 AAAA ATOM 2943 C THR A 367 12.711 26.377 65.166 1.00 33.29 AAAA ATOM 2944 O THR A 367 12.178 23.918 67.352 1.00 30.45 AAAA ATOM 2944 O THR A 367 12.178 23.918 67.352 1.00 30.45 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.05 AAAA ATOM 2947 CB LEU A 368 12.888 25.560 69.482 1.00 32.05 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2949 CDI LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2949 CDI LEU A 368 13.085 26.749 70.421 1.00 32.71 AAAA ATOM 2950 CDZ LEU A 368 13.085 26.749 70.421 1.00 32.71 AAAA ATOM 2950 CDZ LEU A 368 13.085 26.749 70.421 1.00 32.71 AAAA ATOM 2950 CDZ LEU A 368 13.266 23.133 70.489 1.00 33.82 AAAA ATOM 2950 CDZ LEU A 368 13.266 23.133 70.489 1.00 33.82 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CB GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2955 CB GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2955 CB GLU A 369 8.974 24.285 73.451 1.00 41.56 AAAA ATOM 2950 CC GLU A 369 6.957 25.489 73.451 1.00 41.56 AAAA ATOM 2950 CC GLU A 369 6.957 25.489 73.451 1.00 41.56 AAAA ATOM 2956 CG GLU A 369 6.957 25.489 73.451 1.00 37.16 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.00 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.00 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.00 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.56 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 45.55 AAAA ATOM 2966 CD LYS A 370 10.597 20.547 68.567 1.00 38.46 AAAA ATOM 2967 CC LYS A 370 10.586 20.322 65.757 1.00 44.55 AAAA ATOM 2966 CD | | | | | | 8.820 | 25.167 | 67.940 | 1.00 33.05 | AAAA |
| ATOM 2938 N THR A 367 9,473 25.959 67.102 1.00 33.07 AAAA ATOM 2939 CA THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2940 CB THR A 367 11.304 26.719 65.641 1.00 32.28 AAAA ATOM 2941 OG1 THR A 367 12.711 26.377 65.641 1.00 33.29 AAAA ATOM 2942 CG2 THR A 367 11.680 25.044 67.442 1.00 33.29 AAAA ATOM 2943 C THR A 367 11.680 25.044 67.442 1.00 31.71 AAAA ATOM 2944 O THR A 367 11.680 25.044 67.442 1.00 31.71 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.05 AAAA ATOM 2946 CA LEU A 368 11.955 25.896 68.426 1.00 32.05 AAAA ATOM 2947 CB LEU A 368 12.888 25.560 69.482 1.00 32.49 AAAA ATOM 2948 CG LEU A 368 14.097 27.809 69.960 1.00 32.27 AAAA ATOM 2949 CD1 LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2949 CD1 LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2950 CD2 LEU A 368 13.709 28.393 68.597 1.00 33.00 AAAA ATOM 2951 C LEU A 368 13.709 28.393 68.597 1.00 33.00 AAAA ATOM 2952 O LEU A 368 13.266 23.133 70.489 1.00 33.82 AAAA ATOM 2955 CB GLU A 369 11.183 24.285 70.645 1.00 33.82 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 OCE GLU A 369 7.509 24.359 73.541 1.00 41.56 AAAA ATOM 2955 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2956 CG GLU A 369 6.917 23.276 73.571 1.00 37.16 AAAA ATOM 2958 OCE GLU A 369 6.917 23.276 73.571 1.00 37.16 AAAA ATOM 2968 N LYS A 370 10.586 21.788 69.315 1.00 37.16 AAAA ATOM 2968 C LYS A 370 10.586 21.788 69.315 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 10.586 21.788 69.315 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.572 20.025 66.464 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.572 20.025 66.464 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.572 20.025 66.449 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.572 20.025 66.464 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.502 20.235 66.4409 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.502 20.235 66.4409 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.502 20.235 66.4409 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.502 20.235 66.4409 1.00 45.55 AAAA | | | | | | 9.140 | 24.006 | 68.172 | 1.00 33.66 | AAAA |
| ATOM 2939 CA THR A 367 10.684 25.540 66.412 1.00 32.27 AAAA ATOM 2940 CB THR A 367 11.304 26.719 65.641 1.00 32.28 AAAA ATOM 2941 OG1 THR A 367 10.473 27.039 64.520 1.00 30.64 AAAA ATOM 2942 CG2 THR A 367 12.711 26.377 65.166 1.00 33.29 AAAA ATOM 2943 C THR A 367 12.712 26.377 65.166 1.00 31.71 AAAA ATOM 2944 O THR A 367 12.178 23.918 67.352 1.00 30.45 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.05 AAAA ATOM 2946 CA LEU A 368 12.888 25.560 69.482 1.00 32.49 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2949 CD1 LEU A 368 14.097 27.809 69.960 1.00 32.71 AAAA ATOM 2949 CD1 LEU A 368 15.488 27.170 69.899 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.709 28 393 68.597 1.00 31.86 AAAA ATOM 2951 C LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2952 O LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 11.183 24.285 70.645 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 8.974 24.285 70.645 1.00 34.30 AAAA ATOM 2955 CB GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2955 CD GLU A 369 7.509 24.359 73.341 1.00 41.56 AAAA ATOM 2955 CD GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2955 CD GLU A 369 8.974 24.285 72.920 1.00 41.56 AAAA ATOM 2955 CD GLU A 369 8.974 24.285 72.920 1.00 41.56 AAAA ATOM 2955 CD GLU A 369 6.957 25.489 73.341 1.00 41.56 AAAA ATOM 2956 CG GLU A 369 6.957 25.489 73.451 1.00 41.56 AAAA ATOM 2958 OEI GLU A 369 6.957 25.489 73.451 1.00 41.56 AAAA ATOM 2956 CG GLU A 369 6.957 25.489 73.451 1.00 41.56 AAAA ATOM 2956 CG LU A 369 6.957 25.489 73.451 1.00 41.55 AAAA ATOM 2956 CG LU A 369 6.957 25.489 73.451 1.00 41.55 AAAA ATOM 2960 C GLU A 369 6.957 25.489 73.451 1.00 41.55 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.16 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.16 AAAA ATOM 2966 CD LYS A 370 8.092 20.320 65.775 1.00 42.68 AAAA ATOM 2966 CD LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2966 CD LYS A 370 10 | | | N | THR | 367 | 9.473 | 25.959 | 67.102 | | |
| ATOM 2940 CB THR A 367 11.304 26.719 65.641 1.00 32.28 AAAA ATOM 2941 OG1 THR A 367 10.473 27.039 64.520 1.00 30.64 AAAA ATOM 2942 CG2 THR A 367 12.711 26.377 65.166 1.00 33.29 AAAA ATOM 2943 C THR A 367 11.680 25.044 67.442 1.00 31.71 AAAA ATOM 2944 O THR A 367 11.680 25.044 67.442 1.00 30.45 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.05 AAAA ATOM 2946 CA LEU A 368 12.888 25.560 69.482 1.00 32.49 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG LEU A 368 14.097 27.809 69.960 1.00 32.27 AAAA ATOM 2949 CD1 LEU A 368 15.488 27.170 69.899 1.00 32.07 AAAA ATOM 2950 CD2 LEU A 368 13.709 28.393 68.597 1.00 31.86 AAAA ATOM 2951 C LEU A 368 12.455 24.334 70.256 1.00 33.82 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 10.687 23.135 71.375 1.00 36.07 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CG GLU A 369 9.211 23.319 71.748 1.00 34.70 AAAA ATOM 2955 CG GLU A 369 9.211 23.319 71.748 1.00 37.00 AAAA ATOM 2955 CG GLU A 369 9.211 23.319 71.748 1.00 37.16 AAAA ATOM 2959 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 C GLU A 369 6.957 25.489 73.451 1.00 41.74 AAAA ATOM 2956 CG GLU A 369 6.957 25.489 73.451 1.00 41.74 AAAA ATOM 2960 C GLU A 369 6.957 25.489 73.451 1.00 41.56 AAAA ATOM 2966 CD LYS A 370 10.586 21.786 69.315 1.00 37.00 AAAA ATOM 2966 CD LYS A 370 10.586 21.786 69.315 1.00 37.00 AAAA ATOM 2966 CD LYS A 370 8.092 20.320 65.775 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 8.092 20.320 65.775 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 8.092 20.320 65.775 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2966 CD LYS A 3 | | | CA | THR A | 367 | 10.684 | 25.540 | 66.412 | | |
| ATOM 2941 OG1 THR A 367 10.473 27.039 64.520 1.00 30.64 AAAA ATOM 2942 CG2 THR A 367 11.680 25.044 67.442 1.00 31.71 AAAA ATOM 2943 C THR A 367 11.680 25.044 67.442 1.00 31.71 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.05 AAAA ATOM 2946 CA LEU A 368 12.888 25.560 69.482 1.00 32.49 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG LEU A 368 14.097 27.809 69.960 1.00 32.71 AAAA ATOM 2949 CD1 LEU A 368 15.488 27.170 69.899 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.709 28.393 68.597 1.00 31.86 AAAA ATOM 2951 C LEU A 368 13.709 28.393 68.597 1.00 31.86 AAAA ATOM 2952 O LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 11.183 24.285 70.645 1.00 34.30 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 36.07 AAAA ATOM 2955 CG GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CG GLU A 369 8.974 24.285 70.645 1.00 38.71 AAAA ATOM 2955 CG GLU A 369 8.974 24.285 70.645 1.00 38.71 AAAA ATOM 2955 CG GLU A 369 8.974 24.285 70.645 1.00 38.71 AAAA ATOM 2955 CG GLU A 369 8.974 24.285 70.645 1.00 38.71 AAAA ATOM 2955 CG GLU A 369 8.974 24.285 70.645 1.00 37.16 AAAA ATOM 2955 CG GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2955 CG GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2955 CG GLU A 369 6.917 23.276 73.572 1.00 41.56 AAAA ATOM 2950 OEI GLU A 369 6.917 23.276 73.572 1.00 41.74 AAAA ATOM 2950 CC GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.90 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.90 AAAA ATOM 2960 C GLU A 369 6.917 23.276 73.572 1.00 44.54 AAAA ATOM 2960 C GLU A 369 6.917 23.276 73.571 1.00 41.56 AAAA ATOM 2960 C GLU A 369 6.917 23.276 73.575 1.00 44.54 AAAA ATOM 2960 C GLU A 369 6.917 23.276 73.575 1.00 44.55 AAAA ATOM 2960 C GLYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2960 C LYS A 370 10.566 20.604 67.177 1.00 39.96 AAAA ATOM 2960 C LYS A 370 10.966 | | 2940 | CB | THR A | 3 367 | 11.304 | 26.719 | | | |
| ATOM 2943 C THR A 367 11.680 25.044 67.442 1.00 31.71 AAAA ATOM 2944 O THR A 367 12.178 23.918 67.352 1.00 30.45 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.05 AAAA ATOM 2946 CA LEU A 368 12.888 25.560 69.482 1.00 32.49 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG LEU A 368 14.097 27.809 69.960 1.00 32.71 AAAA ATOM 2949 CD1 LEU A 368 15.488 27.170 69.899 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.709 28.393 68.597 1.00 31.86 AAAA ATOM 2951 C LEU A 368 13.709 28.393 68.597 1.00 31.86 AAAA ATOM 2952 O LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 10.687 23.135 71.375 1.00 36.07 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 41.56 AAAA ATOM 2955 CB GLU A 369 7.509 24.359 73.451 1.00 41.56 AAAA ATOM 2959 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OCE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 CC GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.71 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.71 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.71 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.71 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 44.54 AAAA ATOM 2967 CC LYS A 370 8.646 20.532 67.186 1.00 44.55 AAAA ATOM 2967 CC LYS A 370 6.099 19.797 64.409 1.00 45.55 AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA ATOM 2967 CC LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA | | 2941 | OG1 | THR A | 367 | | | | | |
| ATOM 2944 O THR A 367 12.178 23.918 67.352 1.00 30.45 AAAA ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.05 AAAAA ATOM 2946 CA LEU A 368 12.888 25.560 69.482 1.00 32.49 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAAA ATOM 2948 CG LEU A 368 14.097 27.809 69.960 1.00 32.71 AAAA ATOM 2949 CD1 LEU A 368 15.488 27.170 69.899 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.709 28.393 68.597 1.00 31.86 AAAA ATOM 2950 CD2 LEU A 368 12.455 24.334 70.256 1.00 33.82 AAAA ATOM 2951 C LEU A 368 12.455 24.334 70.256 1.00 33.82 AAAA ATOM 2952 O LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 36.07 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 37.16 AAAA ATOM 2955 CB GLU A 369 6.917 23.276 73.572 1.00 41.56 AAAA ATOM 2950 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2961 O GLU A 369 10.893 21.822 70.611 1.00 37.71 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.71 AAAA ATOM 2961 O GLU A 369 10.893 21.822 70.611 1.00 37.71 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 44.54 AAAA ATOM 2967 CE LYS A 370 8.646 20.532 67.186 1.00 44.55 AAAA ATOM 2966 CD LYS A 370 8.692 20.320 65.775 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2967 CE LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2969 C LYS A 370 12.2 | ATOM | 2942 | CG2 | THR A | 367 | | | | | |
| ATOM 2945 N LEU A 368 11.955 25.896 68.426 1.00 32.05 AAAA ATOM 2946 CA LEU A 368 12.888 25.560 69.482 1.00 32.49 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG LEU A 368 14.097 27.809 69.960 1.00 32.71 AAAA ATOM 2949 CD1 LEU A 368 15.488 27.170 69.899 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.709 28.393 68.597 1.00 31.86 AAAA ATOM 2951 C LEU A 368 12.455 24.334 70.256 1.00 33.82 AAAA ATOM 2952 O LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.29 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.30 AAAA ATOM 2955 CB GLU A 369 9.211 23.315 71.375 1.00 36.07 AAAA ATOM 2955 CG GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAAA ATOM 2955 CG GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2957 CD GLU A 369 6.917 23.276 73.572 1.00 41.56 AAAA ATOM 2959 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 C GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 C GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2960 C GLU A 369 6.957 25.489 73.451 1.00 41.74 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2961 C GLU A 369 11.338 20.831 71.196 1.00 37.10 AAAA ATOM 2961 C GLU A 369 11.338 20.831 71.196 1.00 37.10 AAAA ATOM 2960 C GLU A 369 11.338 20.831 71.196 1.00 37.10 AAAA ATOM 2960 C GLU A 369 11.338 20.831 71.196 1.00 37.10 AAAA ATOM 2960 C GLU A 369 11.338 20.831 71.196 1.00 37.10 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 42.68 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 45.55 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 45.55 AAAA ATOM 2967 CE LYS A 370 8.646 20.532 67.186 1.00 45.55 AAAA ATOM 2967 CE LYS A 370 8.092 20.320 65.775 1.00 44.54 AAAA ATOM 2967 CE LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2967 CE LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2969 C LYS A 370 12.683 19. | ATOM | 2943 | С | | | | | | | |
| ATOM 2946 CA LEU A 368 12.888 25.560 69.482 1.00 32.49 AAAA ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG LEU A 368 14.097 27.809 69.960 1.00 32.71 AAAA ATOM 2949 CD1 LEU A 368 15.488 27.170 69.899 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.709 28 393 68.597 1.00 31.86 AAAA ATOM 2951 C LEU A 368 12.455 24.334 70.256 1.00 33.82 AAAA ATOM 2953 N GLU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 10.687 23.135 71.375 1.00 36.07 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2957 CD GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2958 OE1 GLU A 369 6.957 24.359 73.341 1.00 41.56 AAAA ATOM 2959 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 CC GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 CC GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 CC GLU A 369 6.917 20.276 73.572 1.00 41.83 AAAA ATOM 2950 CC GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2960 C GLU A 369 11.338 20.831 71.196 1.00 37.16 AAAA ATOM 2961 C GLU A 369 11.338 20.831 71.196 1.00 37.16 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2966 CD LYS A 370 8.092 20.320 65.775 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 8.092 20.320 65.775 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2966 CD LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2966 CD LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2967 CE LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 6.009 19. | ATOM . | 2944 | 0 | | | | | | | |
| ATOM 2947 CB LEU A 368 13.085 26.749 70.421 1.00 32.27 AAAA ATOM 2948 CG LEU A 368 14.097 27.809 69.960 1.00 32.71 AAAA ATOM 2949 CD1 LEU A 368 15.488 27.170 69.899 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.709 28 393 68.597 1.00 31.86 AAAA ATOM 2951 C LEU A 368 12.455 24.334 70.256 1.00 33.82 AAAA ATOM 2952 O LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.29 AAAA ATOM 2955 CB GLU A 369 10.687 23.135 71.375 1.00 36.07 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.375 1.00 36.07 AAAA ATOM 2956 CG GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2957 CD GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2958 OEI GLU A 369 7.509 24.359 73.341 1.00 41.56 AAAA ATOM 2958 OEI GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 OE GLU A 369 6.957 25.489 73.451 1.00 41.74 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2961 O GLU A 369 11.338 20.831 71.196 1.00 37.00 AAAA ATOM 2961 O GLU A 369 11.338 20.831 71.196 1.00 37.00 AAAA ATOM 2961 O GLU A 369 11.338 20.831 71.196 1.00 37.00 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2966 CD LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2966 CD LYS A 370 8.692 20.320 65.775 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 8.692 20.320 65.775 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.099 19.797 64.409 1.00 45.50 AAAA ATOM 2968 NZ LYS A 370 6.099 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 6.099 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 | ATOM | 2945 | N | LEU A | 368 | | | | | |
| ATOM 2948 CG LEU A 368 14.097 27.809 69.960 1.00 32.71 AAAA ATOM 2940 CD1 LEU A 368 15.488 27.170 69.899 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.709 28 393 68.597 1.00 31.86 AAAA ATOM 2951 C LEU A 368 12.455 24.334 70.256 1.00 33.82 AAAA ATOM 2952 O LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.30 AAAA ATOM 2955 CB GLU A 369 10.687 23.135 71.375 1.00 36.07 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CG GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2955 CD GLU A 369 7.509 24.359 73.341 1.00 41.56 AAAA ATOM 2958 OEI GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2958 OEI GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 CE GLU A 369 6.957 25.489 73.451 1.00 41.74 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2961 O GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2961 O GLU A 369 11.338 20.831 71.196 1.00 37.71 AAAA ATOM 2963 CA LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2963 CA LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2963 CA LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 42.68 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 42.68 AAAA ATOM 2966 CD LYS A 370 6.572 20.075 65.781 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAAA ATOM 2969 C LYS A 370 6.009 19.797 68.493 1.00 37.86 | ATOM | 2946 | CA | | | | | | | |
| ATOM 2949 CD1 LEU A 368 15.488 27.170 69.899 1.00 33.00 AAAA ATOM 2950 CD2 LEU A 368 13.709 28 393 68.597 1.00 31.86 AAAA ATOM 2951 C LEU A 368 12.455 24.334 70.256 1.00 33.82 AAAA ATOM 2952 O LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.30 AAAA ATOM 2954 CA GLU A 369 10.687 23.135 71.375 1.00 36.07 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CG GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2957 CD GLU A 369 7.509 24.359 73.341 1.00 41.56 AAAAA ATOM 2958 OEI GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 CE GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2950 CE GLU A 369 6.957 25.489 73.451 1.00 41.74 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.00 AAAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.00 AAAAA ATOM 2961 CG GLU A 369 10.893 21.822 70.611 1.00 37.00 AAAAA ATOM 2966 CG GLU A 369 10.893 21.822 70.611 1.00 37.00 AAAAA ATOM 2966 CG GLU A 369 10.893 21.822 70.611 1.00 37.00 AAAAA ATOM 2966 CG GLU A 369 10.586 21.788 69.315 1.00 37.71 AAAAA ATOM 2966 CG GLU A 369 10.797 20.547 68.567 1.00 38.46 AAAAA ATOM 2966 CG GLUSA A 370 10.797 20.547 68.567 1.00 38.46 AAAAA ATOM 2966 CG GLUSA A 370 8.646 20.532 67.186 1.00 39.96 AAAAA ATOM 2966 CG GLUSA A 370 8.646 20.532 67.186 1.00 42.68 AAAAA ATOM 2966 CG GLUSA A 370 8.692 20.320 65.775 1.00 44.54 AAAAA ATOM 2966 CD GLUSA A 370 6.572 20.075 65.781 1.00 45.55 AAAAA ATOM 2967 CE GLUSA A 370 6.009 19.797 64.409 1.00 45.55 AAAAA ATOM 2969 C GLUSA A 370 6.009 19.797 64.409 1.00 45.55 AAAAA ATOM 2969 C GLUSA A 370 6.009 19.797 64.409 1.00 45.55 AAAAA ATOM 2967 CE GLUSA A 370 6.009 19.797 64.409 1.00 45.55 AAAAA ATOM 2967 CE GLUSA A 370 6.009 19.797 64.409 1.00 45.55 AAAAA ATOM 2967 CE GLUSA A 370 6.009 19.797 64.409 1.00 45.55 AAAAA ATOM 2967 CE GLUSA A 370 6.009 19.797 64.409 1.00 45.55 AAAAA ATOM 2969 C GLUSA A 370 6.009 19.797 64.409 | ATOM | 2947 | CB | | | • | | | | |
| ATOM 2950 CD2 LEU A 368 13.709 28 393 68.597 1.00 31.86 AAAA ATOM 2951 C LEU A 368 12.455 24.334 70.256 1.00 33.82 AAAA ATOM 2952 O LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.30 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.375 1.00 36.07 AAAA ATOM 2955 CG GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2955 CG GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2957 CD GLU A 369 7.509 24.359 73.341 1.00 41.56 AAAA ATOM 2958 OE1 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OE2 GLU A 369 6.957 25.489 73.451 1.00 41.74 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2961 O GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2962 N LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2963 CA LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2964 CB LYS A 370 10.586 21.788 69.315 1.00 39.96 AAAA ATOM 2965 CG LYS A 370 8.646 20.532 67.186 1.00 42.68 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 42.68 AAAA ATOM 2967 CE LYS A 370 6.572 20.320 65.775 1.00 44.54 AAAA ATOM 2967 CE LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAAA ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAAA AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAAA AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAAA AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAAA AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAAA AAAA ATOM 2969 C LYS A 370 12.683 19.071 68.493 1.00 37.86 | ATOM | 2948 | | | | | | | | |
| ATOM 2951 C LEU A 368 12.455 24.334 70.256 1.00 33.82 AAAA ATOM 2952 O LEU A 368 13.266 23.133 70.489 1.00 34.29 AAAA ATOM 2953 N GLU A 369 11.183 24.285 70.645 1.00 34.30 AAAA ATOM 2955 CB GLU A 369 9.211 23.315 71.375 1.00 36.07 AAAA ATOM 2955 CB GLU A 369 9.211 23.319 71.748 1.00 38.71 AAAA ATOM 2957 CD GLU A 369 8.974 24.285 72.920 1.00 40.18 AAAA ATOM 2958 OEI GLU A 369 7.509 24.359 73.341 1.00 41.56 AAAA ATOM 2959 OE2 GLU A 369 6.917 23.276 73.572 1.00 41.83 AAAA ATOM 2959 OE2 GLU A 369 6.957 25.489 73.451 1.00 41.74 AAAA ATOM 2959 OE2 GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2960 C GLU A 369 10.893 21.822 70.611 1.00 37.16 AAAA ATOM 2961 O GLU A 369 11.338 20.831 71.196 1.00 37.00 AAAA ATOM 2962 N LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2963 CA LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2964 CB LYS A 370 10.586 21.788 69.315 1.00 37.71 AAAA ATOM 2965 CG LYS A 370 8.646 20.532 67.186 1.00 42.68 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 42.68 AAAA ATOM 2966 CD LYS A 370 8.646 20.532 67.186 1.00 44.54 AAAA ATOM 2966 CD LYS A 370 6.572 20.320 65.775 1.00 44.54 AAAA ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.55 AAAA ATOM 2969 C LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA AAAA ATOM 2969 C LYS A 370 12.683 19.071 68.493 1.00 37.86 | MOTA | | | | | | | | | |
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| ATOM 2964 CB LYS A 370 10.166 20.604 67.177 1.00 39.96 AAAA ATOM 2965 CG LYS A 370 8.646 20.532 67.186 1.00 42.68 AAAA ATOM 2966 CD LYS A 370 8.092 20.320 65.775 1.00 44.54 AAAA ATOM 2967 CE LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA ATOM 2969 C LYS A 370 12.683 19.071 68.493 1.00 37.86 | | | CA | | | | | | | |
| ATOM 2965 CG LYS A 370 8.646 20.532 67.186 1.00 42.68 AAAA ATOM 2966 CD LYS A 370 8.092 20.320 65.775 1.00 44.54 AAAA ATOM 2967 CE LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA ATOM 2970 O LYS A 370 12.683 19.071 68.493 1.00 37.86 | | | CB | | | | | | | |
| ATOM 2966 CD LYS A 370 8.092 20.320 65.775 1.00 44.54 AAAA ATOM 2967 CE LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA ATOM 2970 O LYS A 370 12.683 19.071 68.493 1.00 37.86 | | 2965 | CG | | | | | | | |
| ATOM 2967 CE LYS A 370 6.572 20.075 65.781 1.00 45.55 AAAA ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.50 AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA ATOM 2970 O LYS A 370 12.683 19.071 68.493 1.00 37.86 AAAA | | 2966 | CD | LYS A | 370 | | | | | |
| ATOM 2968 NZ LYS A 370 6.009 19.797 64.409 1.00 45.30 AAAA ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA ATOM 2970 O LYS A 370 12.683 19.071 68.493 1.00 37.86 AAAA | | 2967 | CE | | | | | | | |
| ATOM 2969 C LYS A 370 12.282 20.235 68.452 1.00 38.34 AAAA 370M 2970 O LYS A 370 12.683 19.071 68.493 1.00 37.86 AAAA | | 2968 | NZ | LYS A | 370 | | | | | |
| 2970 O LYS A 370 12.683 19.071 68.493 1.00 37.86 AAAA | | 2969 | | LYS ? | 370 | | | | | |
| | | 2970 | 0 | LYS A | A 370 | 12.683 | 19.071 | 68.493 | 1.00 37.86 | AAAA • |

| _ | | | | | | | | | |
|----------------|------|------|-------|------|---------------|--------|---------|--------------|--------|
| ATOM | 2971 | N | ALA A | 371 | 13.105 | 21.266 | 68.311 | 1.00 37.69 | AAAA |
| | 2972 | | | | | | 68.226 | 1.00 37,20 | 2222 |
| MOTA | 2912 | CA | ALA A | | 14.543 | 21.057 | | | AAAA |
| ATOM | 2973 | CB | ALA A | 371 | 15.258 | 22.375 | 67.936 | 1.00 35.48 | AAAA |
| - , | | | | | | | | | |
| MOTA | 2974 | С | ALA A | 371 | 15.023 | 20.477 | 69.558 | 1.00 37.63 | AAAA |
| ATOM | 2975 | 0 | ALA A | 371 | 15.920 | 19.626 | 69.585 | 1.00 37.12 | AAAA |
| | | | | | | | | | |
| MOTA | 2976 | N | LYS A | 372 | 14.426 | 20.930 | 70.665 | 1.00 37.59 | AAAA |
| , | 2027 | CX | LYS A | 272 | 14.796 | 20,432 | .71.995 | 1.00 37.46 | AAAA |
| ATOM | 2977 | CA | | | 14.790 | | | | |
| MOTA | 2978 | CB | LYS A | 372 | 14.022 | 21.156 | 73.095 | 1.00 36.52 | AAAA |
| | - | | | | | | | | |
| MOTA | 2979 | CG | LYS A | 3/2 | 14.287 | 22.634 | 73.111 | 1.00 22.67 | AAAA |
| MOTA | 2980 | CD | LYS A | 372 | 13.309 | 23.396 | 74.022 | 1.00 22.67 | AAAA |
| AION | | | | | | | | | |
| MOTA | 2981 | CE | LYS A | 372 | 13.600 | 24.874 | 73.901 | 1.00 22.67 | AAAA |
| | | RTFT | LYS A | 272 | 12.692 | 25.708 | 74.785 | 1.00 22.67 | AAAA |
| MOTA | 2982 | NZ | | | | | | | |
| MOTA | 2983 | C | LYS A | 372 | 14.495 | 18.957 | 72.077 | 1.00 37.60 | AAAA . |
| | | | | | | | | | |
| ATOM | 2984 | 0 | LYS A | 3/2 | 15.367 | 18.171 | 72.407 | 1.00 37.26 | AAAA |
| MOTA | 2985 | N | ALA A | 777 | 13.249 | 18.595 | 71.789 | 1.00 38.17 | AAAA |
| | | | | | | | | | |
| ATOM | 2986 | CA | ALA A | 3/3 | 12.812 | 17.206 | 71.829 | 1.00 39.55 | AAAA |
| ATOM | 2987 | CB | ALA A | 377 | 11.365 | 17.109 | 71.395 | 1.00 39.34 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2988 | С | ALA A | 373 | 13.675 | 16.277 | 70.972 | 1.00 41.02 | AAAA |
| | | 0 | ALA A | | 14.366 | 15.410 | 71.561 | 1.00 42.26 | AAAA |
| MOTA | 2989 | U | | | | | | | |
| MOTA | 2990 | TXO | ALA A | 373 | 13.663 | 16.416 | 69.725 | 1.00 42.06 | AAAA |
| | | | | | | | | | |
| HETATM | Z991 | ZN | ZN B | 951 | 23.696 | 34.788 | 54.072 | 1.00 27.38 | ZONE |
| HETATM | 2992 | 01 | SHA C | 1 | 24.578 | 33.295 | 53.458 | 1.00 31.95 | SAHA |
| | | | | | | | | | |
| HETATM | 2993 | 02 | SHA C | 1 | 24.294 | 35:218 | 51.444 | 1.00 33.51 | Saha |
| HETATM | 2004 | N1 | SHA C | 1 | 24.578 | 33.085 | 52.069 | 1.00 34.03 | SAHA |
| | | | | | | | | | |
| HETATM | 2995 | C1 | SHA C | 1 | 24.063 | 34.053 | 51.246 | 1.00 34.25 | SAHA |
| HETATM | | | SHA C | 1 | 23.090 | 33.625 | 50.259 | 1.00 36.87 | SAHA. |
| HETATM | 2990 | C2 | | | | | | | |
| HETATM | 2997 | C3 | SHA C | 1 | 23.548 | 33.781 | 48.816 | 1.00 39.33 | SAHA |
| | | | SHA C | 1 | • | 33.274 | 47.852 | 1.00 40.86 | SAHA |
| HETATM | | C4 | SHA C | | 22.498 | | | | |
| HETATM | 2999 | C5 | SHA C | 1 | 21.590 | 34.413 | 47.455 | 1.00 43.37 | SAHA |
| | | | | | | | 46.092 | 1.00 46.72 | |
| HETATM | 3000 | C6 | SHA C | 1 | 21.061 | 34.017 | | | SAHA |
| HETATM | 3001 | C7 | SHA C | 1 | 19.754 | 34.714 | 45.787 | 1.00 48.75 | Saha |
| | | | | | | | | | |
| HETATM | 3002 | C8 | SHA C | 1 | 19.960 | 35.720 | 44.693 | 1.00 50.75 | SAHA |
| HETATM | 3003 | 03 | SHA C | 1 | 20.381 | 35.467 | 43.575 | 1.00 51.08 | SAHA |
| | | | | | | | | | |
| HETATM | 3004 | N2 | SHA C | 1 | 19.591 | 36.956 | 45.085 | 1.00 52.52 | SAHA |
| HETATM | | C9 | SHA C | 1 | 19.842 | 38.330 | 44.507 | 1.00 54.25 | SAHA |
| | | | | | | | | | |
| HETATM | 3006 | C10 | SHA C | 1 | 19.243 | 39.431 | 45.215 | 1.00 55.76 | SAHA |
| | | C1 1 | SHA C | 1 | 19.423 | 40.804 | 44.727 | 1.00 56.53 | SAHA |
| HETATM | | | | | | | | | |
| HETATM | 3008 | C12 | SHA C | 1 | 20.169 | 41.085 | 43.545 | 1.00 56.58 | SAHA |
| | | | | | | | 42.827 | 1.00 55.93 | SAHA |
| HETATM | 3009 | CIS | SHA C | 1 | 20.755 | 39.942 | | | |
| HETATM | 3010 | C14 | SHA C | 1 | 20.612 | 38.546 | 43.304 | 1.00 54.65 | Saha |
| | | | | | | | 49.378 | 1.00 4.67 | SOLV |
| HETATM | 3011 | UHZ | WAT D | 2 | 36.485 | 44.023 | | | |
| HETATM | 3012 | OH2 | WAT D | 3 | 27.702 | 16.865 | 62.162 | 1.00 4.67 | SOLV |
| | | | | | | | 59.575 | 1.00 10.12 | |
| HETATM | 2072 | OHZ | WAT D | 4 | 23.251 | 30.387 | | | SOLV |
| HETATM | 3014 | OH2 | WAT D | 5 | 33.825 | 41.862 | 46.926 | 1.00 21.13 | SOLV |
| | | | | | | | 47.867 | | |
| HETATM | 20T2 | OH2 | WAT D | 6 | 24.866 | 44.453 | 47.007 | 1.00 23.72 | SOLV |
| H TATM | 3016 | OH2 | WAT D | 7 | 34.145 | 20.442 | 33.590 | 1.00 18.19 | SOLV |
| | | | | | | | | | |
| HLTATM | 3017 | OH2 | WAT D | 8 | 7.921 | 29.753 | 62.099 | 1.00 20.79 | SOLV |
| H_ TATM | | OH2 | WAT D | 9 | 17.863 | 6.978 | 64.018 | 1.00 28.94 | SOLV |
| | | | | | | | | | |
| HETATM | 3019 | OH2 | WAT D | 10 | 35.580 | 44.610 | 74.823 | 1.00 31.62 | SOLV |
| HETATM | 3020 | OH2 | WAT D | 11 | 49.208 | 27.797 | 65.303 | 1.00 14.70 | SOLV |
| | | | | | | | | | |
| HETATM | 3021 | OH2 | WAT D | 12 | 20.490 | 34.049 | 61.067 | 1.00 25.01 | SOLV |
| HETATM | | OHO | WAT D | 13 | 44.757 | 33.106 | 46.084 | 1.00 25.90 | SOLV |
| | | | | | | | | | |
| HETATM | 3023 | OH2 | WAT D | 14 | 22.457 | 60.823 | 57.444 | 1.00 15.21 | SOLV |
| HETATM | | OH2 | | 15 | 3.399 | 32.742 | 65.163 | 1.00 20.66 | SOLV |
| HETAIM | 3024 | | | | | | | | |
| HETATM | 3025 | OH2 | WAT D | 16 | 32.273 | 51.414 | 45.610 | 1.00 22.37 | SOLV |
| | 2026 | | WAT D | | 26.328 | 42.873 | 73.427 | 1.00 27.86 | SOLV |
| · HETATM | | | | 17 | | | | | |
| HETATM | 3027 | OH2 | WAT D | 18 | 48.249 | 24.121 | 56.778 | 1.00 15.09 | SOLV |
| | | | | | | | 72.082 | 1.00 40.95 | SOLV |
| HETATM | 3028 | OH2 | WAT D | 19 | 15.249 | 44.552 | | | |
| HETATM | 3029 | OH2 | WAT D | 20 | 26.444 | 9.269 | 52.633 | 1.00 26.66 | SOLV |
| UPIWIN | 3023 | | | | | | | | |
| HETATM | 3030 | OH2 | WAT D | 21 | 26.554 | 18.383 | 59.650 | 1.00 11.42 | SOLV |
| HETATM | 3031 | он2 | WAT D | 22 . | 39.456 | 25.964 | 72.316 | 1.00 20.32 | SOLV |
| HETATM | 2027 | | | | | | | | |
| HETATM | 3032 | OH2 | WAT D | 23 | 26.743 | 37.600 | 38.359 | 1.00 37.22 | SOLV |
| | 2022 | OH2 | | 24 | 44.666 | 23.818 | 39.068 | 1.00 32.27 | SOLV |
| HETATM | 2022 | | | | | | | | |
| HETATM | 3034 | OH2 | WAT D | . 25 | 14.714 | 52.213 | 70.663 | 1.00 29.24 | SOLV |
| IIII I FI A FA | 2025 | 0112 | MAM D | | | | 69.864 | 1.00 29.58 | SOLV |
| HETATM | 3035 | Onz | WAT D | 26 | 45.129 | 18.856 | | | |
| HETATM | 3036 | OH2 | WAT D | 27 | 30.024 | 17.886 | 49.758 | 1.00 15.52 | SOLV |
| 11111111111 | 2000 | | · | • | | | • | - | • |
| | | | | | | | | | |

| HETATM | 3037 | OH2 | WAT | D | 28 | 20.659 | 28.788 | 43.520 | 1.00 28.55 | SOLV |
|----------|------|------|------|---|------|--------|--------|--------|------------|------|
| HETATM | 3038 | OH2 | WAT | D | 29 | 32.271 | 38.000 | 53.512 | 1.00 47.72 | SOLV |
| HETATM | 3039 | OH2 | WAT | D | 30 | 18.285 | 29.333 | 54.536 | 1.00 21.34 | SOLV |
| HETATM | 3040 | OH2 | WAT | D | 31 | 49.978 | 38.669 | 73.461 | 1.00 31.02 | SOLV |
| HETATM | 3041 | OH2 | WAT | D | 32 | 21.587 | 50.3B6 | 71.043 | 1.00 14.52 | SOLV |
| HETATM | 3042 | OH2 | WAT | D | 33 | 46.784 | 32.121 | 33.375 | 1.00 31.79 | SOLV |
| HETATM | | OH2 | WAT | D | 34 | 33.359 | 39.755 | 49.117 | 1.00 16.13 | SOLV |
| HETATM | | | WAT | | 35 | 7.687 | 37.657 | 51.568 | 1.00 27.22 | SOLV |
| HETATM | | | WAT | | 36 | 44.238 | 35.392 | 33.961 | 1.00 19.67 | SOLV |
| HETATM | | | WAT | | 37 | 10.908 | 25.384 | 58.206 | 1.00 33.51 | SOLV |
| HETATM | | | WAT | | 38 | 36.758 | 27.243 | 70.552 | 1.00 39.61 | SOLV |
| HETATM | | | WAT | | 39 | 45.825 | 46.691 | 54.654 | 1.00 32.43 | SOLV |
| . HETATM | | | WAT | | 40 | 52.489 | 20.282 | 52.165 | 1.00 39.37 | SOLV |
| HETATM | | | WAT | | 42 | 12.117 | 17.831 | 56.596 | 1.00 27.74 | SOLV |
| HETATM | | | WAT | | . 43 | 45.023 | 26.168 | 35.172 | 1.00 27.74 | |
| | | | WAT | | 44 | 39.392 | 12.771 | 62.066 | | SOLV |
| HETATM | • | | | | | 3,930 | 26.970 | | 1.00 35.15 | SOLV |
| HETATM | | | WAT | | 45 | | | 63.814 | 1.00 22.23 | SOLV |
| HETATM | | | WAT | | 46 | 8.454 | 19.321 | 71.677 | 1.00 32.36 | SOLV |
| HETATM | | | WAT | | 47 | 20.280 | 18.126 | 73.237 | 1.00 33.88 | SOLV |
| HETATM | | | TAW | | 48 | 9.321 | 39.409 | 54.873 | 1.00 18.57 | SOLV |
| HETATM | | | WAT | | 49 | 50.852 | 41.323 | 58.048 | 1.00 21.25 | SOLV |
| HETATM | | | WAT | | 50 | 37.134 | 34.599 | 60.315 | 1.00 61.70 | SOLV |
| HETATM | | | WAT | | 51 | 14.944 | 62.815 | 48.613 | 1.00 42.50 | SOLV |
| HETATM | | | WAT | | 52 | 6.494 | 33.164 | 51.420 | 1.00 40.65 | SOLV |
| HETATM | | | WAT | | 53 | 24.913 | 44.799 | 72.298 | 1.00 17.10 | SOLV |
| HETATM | | | WAT | | 54 | 51.156 | 35.095 | 48.814 | 1.00 23.05 | SOLV |
| HETATM | | | TAW | | 55 | 16.518 | 41.750 | 45.596 | 1.00 49.25 | SOLV |
| HETATM | | | WAT | | 56, | 10.326 | 16.413 | 61.267 | 1.00 46.03 | SOLV |
| HETATM | | | WAT | | 57 | 25.316 | 47.708 | 73.062 | 1.00 22.73 | SOLV |
| HETATM | | - | WAT | | 58 | 4.013 | 33.865 | 76.173 | 1.00 44.82 | SOLV |
| HETATM | | | TAW | | 59 | 24.846 | 18.072 | 36.805 | 1.00 34.67 | SOLV |
| HETATM | | | WAT | | 60 | 15.930 | 56.853 | 61.737 | 1.00 55.56 | SOLV |
| HETATM | | | WAT | | 61 | 49.662 | 44.249 | 48.982 | 1.00 28.72 | SOLV |
| HETATM | | | WAT | | 62. | 23.232 | 17.421 | 53.920 | 1.00 13.11 | SOLV |
| HETATM | | | WAT | | 63 | 39.293 | 23.035 | 33.289 | 1.00 35.79 | SOLV |
| HETATM | | | WAT | | 64 | 19.908 | 20.169 | 44.339 | 1.00 24.33 | SOLV |
| HETATM | | | TAW | | 65 | 33.259 | 21.655 | 69.560 | 1.00 45.10 | SOLV |
| HETATM | | | WAT | | 66 | 27.528 | 53.947 | 68.629 | 1.00 44.79 | SOLV |
| HETATM | | | TAW | | 67 | 18.774 | 48.716 | 52.865 | 1.00 54.01 | SOLV |
| HETATM | | | TAW | | 68 | 10.877 | 29.062 | 63.401 | 1.00 27.08 | SOLV |
| HETATM | | | WAT | | 69 | 43.057 | 31.367 | 28.786 | 1.00 30.16 | SOLV |
| HETATM | | | WAT | | 70 | 24.816 | 44.057 | 43.447 | 1.00 20.11 | SOLV |
| HETATM | | | | | 71 | 37.368 | 38.823 | 46.381 | 1.00 33.55 | SOLV |
| HETATM | | | WAT | | 72 | 9.038 | 18.327 | 63.519 | 1.00 31.34 | SOLV |
| HETATM | | | WAT | | 73 | 51.799 | 20.829 | 65.265 | 1.00 28.32 | SOLV |
| HETATM | | | TAW | | 74 | 17.556 | 58.515 | 57.254 | 1.00 19.27 | SOLV |
| HETATM | | | WAT | | 75 | 28.436 | 27.904 | 79.425 | 1.00 27.13 | SOLV |
| HETATM | | | WAT | | 76 | 18.939 | 35.798 | 35.800 | 1.00 94.18 | SOLV |
| HETATM | 3085 | | WAT | | 77 | 34.359 | 31.251 | 46.688 | 1.00 73.70 | SOLV |
| HETATM | | | WAT | | 78 | 44.373 | 51.649 | 60.029 | 1.00 30.23 | SOLV |
| METATM | 3087 | OH2 | WAT | D | 79 | 28.537 | 63.478 | 48.324 | 1.00 21.09 | SOLV |
| HETATM | 3088 | OH2 | WAT | D | 80 | 6.869 | 44.113 | 72.030 | 1.00 28.59 | SOLV |
| HETATM | 3089 | | WAT | | 81 | 42.882 | 18.761 | 71.115 | 1.00 31.80 | SOLV |
| HETATM | 3090 | OH2 | TAW | D | 82 | 36.712 | 59.078 | 53.901 | 1.00 40.11 | SOLV |
| HETATM | 3091 | OH2 | TAW | D | 83 | 37.506 | 42.495 | 40.104 | 1.00 51.37 | SOLV |
| HETATM | 3092 | OH2 | WAT | D | 84 | 40.054 | 38.439 | 55.415 | 1.00 20.07 | SOLV |
| HETATM | 3093 | OH2 | WAT | D | 85 | 32.170 | 56.633 | 72.920 | 1.00 45.23 | SOLV |
| HETATM | 3094 | | WAT | | 86 | 24.470 | 53.877 | 47.119 | 1.00 41.18 | SOLV |
| HETATM | | | WAT | | 87 | 48.585 | 35.663 | 67.518 | 1.00 33.40 | SOLV |
| HETATM | | | WAT | | 88 | 29.541 | 57.166 | 42.788 | 1.00 44.61 | SOLV |
| HETATM | | | WAT | | 89 | 47.814 | 28.707 | 41.228 | 1.00 45.64 | SOLV |
| HETATM | | | WAT | | 90 | 49.377 | 52.112 | 63.320 | 1.00 22.26 | SOLV |
| HETATM | | | TAW | | 91 | 44.219 | 43.589 | 43.912 | 1.00 39.90 | SOLV |
| HETATM | 3100 | | WAT | | 92 | 25.913 | 61.639 | 75.382 | 1.00 48.28 | SOLV |
| HETATM | 3101 | | WAT | | 93 | 8.623 | 30.749 | 49.707 | 1.00 40.37 | SOLV |
| | | | WAT | | 94 | 45.634 | 41.080 | 40.990 | 1.00 21.46 | SOLV |
| HETATM | 2102 | 0.12 | **** | _ | | | | | | |

SUBSTITUTE SHEET (RULE 26)

| HETATM | 3103 | OH2 | WAT | D | 95 | | 29.984 | 34.886 | 51.725 | 1.00 | 35.75 | SOLV |
|--------|------|------|----------------------------------|---|-----|---|--------|--------|-----------------|------|-------|-------|
| HETATM | | OH2 | TAW | D | 96 | | 13.051 | 21.934 | 49.804 | 1.00 | 46.73 | SOLV |
| HETATM | | OH2 | WAT | D | 97 | | 32.412 | 65.913 | 55.822 | 1.00 | 43.39 | SOLV |
| HETATM | | | TAW | | 98 | | 35.056 | 43.390 | 38.348 | 1.00 | 34.53 | SOLV |
| HETATM | | OH2 | WAT | D | 99 | | 22.360 | 47.680 | 60.688 | 1.00 | 19.16 | SOLV |
| HETATM | | | WAT | | | | 50.755 | 19.722 | 57.906 | 1.00 | 42.45 | SOLV |
| HETATM | | | WAT | | | | 7.875 | 37.690 | 74.094 | 1.00 | | SOLV |
| HETATM | 3110 | | WAT | | | | 24.080 | 26.796 | 43.617 | 1.00 | | SOLV |
| | | | WAT | | | | 45.206 | 34.126 | 75.765 | 1.00 | | SOLV |
| HETATM | | | WAT | | | | 26.110 | 54.786 | 40.685 | 1.00 | | SOLV |
| HETATM | | | WAT | | | | 25.918 | 39.658 | 77.647 | 1.00 | | SOLV |
| HETATM | 3113 | | | | | - | 41.578 | 18.191 | 36.809 | 1.00 | | SOLV |
| HETATM | 3114 | | TAW | | | | | 51.420 | 73.896 | 1.00 | | SOLV |
| HETATM | | | TAW | | | | 31.945 | | | | | |
| HETATM | | | WAT | | | | 16.722 | 60.311 | 51.182 | | 48.74 | SOLV |
| HETATM | | | WAT | | | | 43.604 | 38.573 | 78.141 | 1.00 | | SOLV |
| HETATM | | | TAW | | | | 16.063 | 15.496 | 69.430 | | 55.36 | SOLV |
| HETATM | | | WAT | | | | 21.630 | 22.785 | 49.145 | 1.00 | | SOLV |
| HETATM | 3120 | | TAW | | | | 27.479 | 56.647 | 44.026 | 1.00 | | SOĻV |
| HETATM | 3121 | OH2 | TAW | D | 113 | | 14.739 | 51.674 | 61.674 | | 35.55 | SOLV |
| HETATM | 3122 | OH2 | WAT | D | 114 | | 50.063 | 26.435 | 54.358 | | 50.86 | SOLV |
| HETATM | | | WAT | | | | 43.935 | 38.427 | 73.129 | | 44.21 | SOLV |
| HETATM | | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | D | 116 | | 49.707 | 31.478 | 5 7. 709 | | 36.11 | SOLV |
| HETATM | | OH2 | WAT | D | 117 | | 25.032 | 43.463 | 55.676 | 1.00 | 38.06 | SOLV |
| HETATM | | OH2 | WAT | D | 118 | | 10.618 | 46.623 | 59.838 | 1.00 | 26.33 | SOLV |
| HETATM | 3127 | OH2 | T'AW | D | 119 | | 48.466 | 33.382 | 61.437 | 1.00 | 19.82 | SOLV |
| HETATM | | OH2 | TAW | D | 120 | | 44.157 | 40.058 | .37.907 | 1.00 | 42.95 | SOLV |
| HETATM | | OH2 | WAT | D | 121 | | 51.267 | 29.446 | 52.889 | 1.00 | 38.93 | SOLV |
| HETATM | | | TAW | | | | 16.653 | 15.228 | 72.975 | 1.00 | 45.41 | SOLV |
| HETATM | | OH2 | TAW | D | 123 | , | 36.898 | 45.148 | 41.936 | 1.00 | 27.00 | SOLV |
| HETATM | | OH2 | WAT | D | 124 | | 49.655 | 34.591 | 59.117 | 1.00 | 38.97 | SOLV |
| HETATM | | | TAW | | | | 12.285 | 57.594 | 42.107 | 1.00 | 23.56 | SOLV |
| HETATM | | | WAT | | | | 28.294 | 57.644 | 73.289 | 1.00 | 34.79 | SOLV |
| HETATM | | | WAT | | | | 19.138 | 60.403 | 61.551 | 1.00 | 28.58 | SOLV |
| HETATM | | | TAW | | | | 30.300 | 33.685 | 34.047 | 1.00 | 27.37 | SOLV |
| HETATM | | | WAT | | | | 40.898 | 53.983 | 47.254 | 1.00 | 16.30 | SOLV |
| HETATM | | | WAT | | | | 43.550 | 32.160 | 38.272 | 1.00 | 38.86 | SOLV |
| HETATM | | | WAT | | | | 18.624 | 13.959 | 56.194 | 1.00 | 37.70 | SOLV. |
| HETATM | | | WAT | | | | 18.580 | 12.901 | 62.894 | 1.00 | 27.28 | SOLV |
| HETATM | | | WAT | | | | 35.830 | 30.296 | 50.621 | 1.00 | 42.47 | SOLV |
| HETATM | | OH2 | WAT | ח | 134 | | 51.219 | 35.855 | 51.878 | 1.00 | 20.37 | SOLV |
| HETATM | | | WAT | | | | 50.428 | 22.486 | 49.267 | | 39.37 | SOLV |
| | | | WAT | | | | 51.633 | 29.369 | 63.918 | | 33.99 | SOLV |
| HETATM | | | WAT | | | | 46.384 | 43.924 | 55.825 | | 22.63 | SOLV |
| HETATM | | | WAT | | | | 30.356 | 25.767 | 28.762 | | 25.84 | SOLV |
| HETATM | 3140 | | WAT | | | | 25.070 | 47.842 | 60.819 | | 25.00 | SOLV |
| HETATM | | | WAT | | | | 47.097 | 49.394 | 69.367 | | 30.58 | SOLV |
| HETATM | | 7112 | WAT | ב | 1/1 | | 15.246 | 37.581 | 73.398 | | 36.82 | SOLV |
| HETATM | | OM2 | WAT | ב | 142 | | 8.341 | 23.099 | 64.695 | | 35.89 | SOLV |
| HETATM | | JH2 | WAT | 7 | 1/2 | | 30.065 | 18.220 | 46.048 | | 14.26 | SOLV |
| HETATM | | VH2 | MWT. | 7 | 144 | | | 46.453 | 57.606 | | 36.15 | SOLV |
| HETATM | 3152 | OH2 | WAT | ע | 744 | | 11.930 | 40.403 | 57.000 | 1.00 | 20.13 | 2010 |

INTERNATIONAL SEARCH REPORT

International application No. PCT/US00/24700

| A. CLASSIFICATION OF SUBJECT MATTER IPC(7): COTK 14/00; GOIN 53/573 US CL: Please See Extra Sheet. According to International Patent Classification (IPC) or to both national classification and IPC B. FIELDS SEARCHED Minimum documentation searched (classification system followed by classification symbols) U.S.: Please See Extra Sheet. Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) Please See Extra Sheet. | | | | | | | | |
|---|--|--|--|--|--|--|--|--|
| C. DOCUMENTS CONSIDERED TO BE RELEVANT | | | | | | | | |
| Category* Citation of document, with indicate | ation, where appropriate, of the relevant passages Relevant to claim No. | | | | | | | |
| Human Heparan Sulfate N Journal of Biological Cher | ucture of the Sulfotransferase Domain of -Deacetylase/N-Sulfotransferase 1. The mistry. 16 April 1999, Volume 274, 0676, see especially the abstract. | | | | | | | |
| of human heparan sulfate | f Lys-614 in the sulfotransferase activity N-deacetulase/N-sulfotransferase. FEBS 3, pages 211-214, see especially the | | | | | | | |
| X Further documents are listed in the continu | ustion of Box C. See patent family space | | | | | | | |
| Special estagories of cited documents: | Further documents are listed in the continuation of Box C. See patent family annex. Special categories of cited documents: Inter document published after the international filing date or priority. | | | | | | | |
| "A" document defining the general state of the art which to be of particular relevance | date and not in conflict with the application but cited to understand | | | | | | | |
| "E" carlier document published on or after the internation "L" document which may throw doubts on priority claim cited to establish the publication date of another of special reason (as specified) | earlier document published on or after the international filing date document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified) "Y" document of particular relevance; the claimed invention cannot be considered novel or caunot be considered to involve an inventive step when the document is taken alone "Ocument of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is taken alone "Ocument of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is taken alone "Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is taken alone "Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is taken alone "Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is taken alone | | | | | | | |
| document published prior to the international filing date but later "&" document member of the same patent family than the priority date claimed | | | | | | | | |
| Date of the actual completion of the international search Date of mailing of the international search report 25 JAN 2001 | | | | | | | | |
| Name and mailing address of the ISA/US Commissioner of Patents and Trademarks Box PCT Washington, D.C. 20231 Facsimile No. (703) 305-3230 | Authorized officer ARDIN MARSOHEL Telephone No. (705) 308-0196 | | | | | | | |

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US00/24700

| | | 17US00/247 | ••• | |
|-------------|---|------------|----------------------|--|
| C (Continua | tion). DOCUMENTS CONSIDERED TO BE RELEVANT | | | |
| Category* | Citation of document, with indication, where appropriate, of the relevant pa | issages | Relevant to claim No | |
| Y | AHMAD et al. WD Repeats of the p48 Subunit of Chicken Chromatin Assembly Factor-1 Required for in Vitro Interact with Chicken Histone Deacetylase-2. The Journal of Biolog Chemistry. 04 June 1999, Volume 274, Number 23, pages 16 16653, see especially the abstract. | 1-19 | | |
| Y | JOHN et al. Rhizobium NodB protein involved in nodulating signal synthesis is a chitooligosaccharide deacetylase. Proce of the National Academy of Sciences, USA. January 1993, 90, pages 625-629, see especially the abstract. | edings | 1-19 | |
| A | US 5,780,594 A (CARTER) 14 July 1998, see the entire disc | losure. | 1-19 | |
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INTERNATIONAL SEARCH REPORT

International application No. PCT/US00/24700

A. CLASSIFICATION OF SUBJECT MATTER: US CL $\,:\,$

530/350 and 435/7.9

B. FIELDS SEARCHED
Minimum documentation searched
Classification System: U.S.

530/300,333,350; 435/6,7.2; 514/2

B. FIELDS SEARCHED

Electronic data bases consulted (Name of data base and where practicable terms used):

CAS, BIOTECH ABS, MEDLINE, EMBASE, WPI, WEST covering search terms: deacetylase, human, crystal, histone, inhibitor, x-ray, and crystallography

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